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Uporaba gladilnih funkcij za glajenje podatkov podanih v diskretni obliki

Using Spline Functions to Smooth Discrete Data

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V prispevku je predstavljen algoritem za izračun gladilnih funkcij, uporabljen v programskem paketu "SPLINE", razvitem v Centru za eksperimentalno mehaniko na Fakulteti za strojništvo v Ljubljani. Podana je podrobna analiza vpliva števila izbranih podintervalov in števila diskretnih vrednosti na natančnost približka. Uporabnost algoritma je prikazana na eksperimentalnih podatkih za realno in imaginarno komponento modula lezenja poli-izobutilena. Podatki, ki smo jih analizirali, so povzeti iz objave [5].

(Ključne besede: funkcije gladilne, glajenje podatkov, algoritmi, paketi programski, SPLINE)

In this paper we present an algorithm for calculating spline functions. This algorithm is integrated into the software package "SPLINE". The influence of the number of pre-selected sub-intervals and the number of datum points per sub-interval on the accuracy of the approximation was analyzed. The power of the algorithm was demonstrated on the shear storage and the loss-compliance data for an uncrosslinked poly-isobutylene. The experimental data were measured and discussed by [5].

(Keywords: spline functions, smoothing splines, algorithms, software packages, SPLINE)

0 UVOD

Rezultat meritev je po navadi množica točk, ki podaja odvisnost med dvema fizikalnima veličinama, recimo *x* in *y*. Zelo pogosto želimo izmerjeno množico točk nadomestiti (približati) z množico diskretnih točk, ki pomenijo "gladko" krivuljo. Ena izmed možnosti, ki jo v praksi pogosto uporabljamo, je približek s polinomom ustreznega reda. Ta postopek bo praviloma dal zadovoljivo rešitev samo v tistih primerih, pri katerih je odvisnost med fizikalnima veličinama *x* in *y* v resnici potenčnega tipa. V vseh drugih primerih (tj., ko je odvisnost eksponentna ali trigonometrična) je omenjeni postopek po navadi nesprejemljiv. V takih primerih najučinkoviteje opravimo postopek glajenja z uporabo zlepkov polinomov tretjega reda.

V prispevku je predstavljen algoritem, ki omogoča interaktivno spreminjanje širine posameznega zlepka, kar omogoča kakovostnejše glajenje eksperimentalnih podatkov z večjim raztrosom. Algoritem je bil uporabljen v programskem paketu 'SPLINE', ki smo ga razvili v Centru za eksperimentalno mehaniko na Fakulteti za strojništvo v Ljubljani za potrebe vrednotenja časovno odvisnega obnašanja polimernih in kompozitnih materialov.

0 INTRODUCTION

The results of measurements are usually given as a set of datum points, which defines the relation between the two measured physical quantities, i.e., *x* and *y*. Very often we want to replace the set of measured data points with a set of discrete data points representing a smooth curve. One of the possible choices we often use in practice is an approximation with polynomials of the appropriate order. This approach would only result in a satisfying solution when the relationship between the physical quantities *x* and *y* is indeed polynomial. In all other cases (i.e., when the relation is exponential or trigonometric) the polynomial approach can be unacceptable. In such cases, the most effective procedure for smoothing the data is the use of so-called "spline" functions.

We present an algorithm that was used in the development of the "SPLINE" computer program at the Center for Experimental Mechanics, Faculty of Mechanical Engineering, University of Ljubljana. The algorithm was used to evaluate the time-dependent behavior of polymers and composite materials.

0.1 Definicija problema

V ravnini $x-y$ naj bo podanih N parov diskretnih vrednosti:

$$\mathcal{F} = \{x_i, y_i;\ i = 1,\ 2,\ ....,\ N;\ N > 3\} \quad (1),$$

ki podajajo odvisnost med izmerjenima fizikalnima veličinama x in y. Diskretne vrednosti naj bodo urejene tako, da bo izpolnjen pogoj:

$$x_i < x_{i+1} \quad (2)$$

za vsak i, ki zadosti pogoju:

$$1 \le i \le N-1 \quad (3).$$

Cilj, ki si ga zastavljamo, je določitev 'gladke' krivulje, ki bo najbolje približala omenjeno odvisnost ne glede na to, kakšna je oblika te odvisnosti.

0.1 Problem statement

In the plane $x-y$ we have a set of N discrete data pairs:

(1),

which defines the relationship between the two measured physical quantities, x and y. Let the discrete values be ordered such that

(2)

for every i, which fulfills the condition

(3).

The goal is to obtain a smooth curve that would faithfully represent the actual relationship between the two physical variables independently of the shape of the underlying relation.

1 TEORETIČNE OSNOVE

Gladilna funkcija je v bistvu krivulja, ki je sestavljena iz množice polinomov tretjega reda. Zaprto območje na osi x, znotraj katerega so podane diskretne vrednosti x_i in y_i, razdelimo na ustrezno število korakov. Znotraj vsakega koraka izvedemo nato približek podanih diskretnih vrednosti s polinomom tretjega reda. Ker zahtevamo, da je približna krivulja zvezna in zvezno odvedljiva, morajo polinomi na stičišču dveh korakov imeti enaki funkcijski vrednosti ter enak prvi in drugi odvod.

1.1 Definicija vozlišč

Zaprto območje:

$$I\left[x_1, x_N\right] \quad (4)$$

razdelimo na K–1 korakov:

$$I_j = \left[t_j, t_{j+1}\right]; \quad j = 1, 2, 3, ..., K-1 \quad (5),$$

kjer sta t_j in t_{j+1} spodnja in zgornja meja j-tega koraka. Velikost j-tega koraka je potem:

$$l_j = t_{j+1} - t_j \quad (6).$$

Meje korakov podaja množica točk:

1 THEORETICAL BACKGROUND

The spline function is essentially a curve assembled from a number of third-order polynomials. The closed interval on the x-axis, within which the discrete values x_i and y_i are given, is divided into an appropriate number of sub-intervals. Within each of the sub-intervals an approximation of the given discrete values is achieved with the third-order polynomials. The approximation curve has to be continuous and continuously derivative. Thus, the value of the polynomials, and their first and second derivatives in the connection points of the two neighboring sub-intervals should have the same values.

1.1 Definition of the connection points

The closed interval:

(4)

we divide into K–1 sub-intervals,

(5),

where t_j and t_{j+1} are the lover and the upper boundary of the j-th sub-interval. Thus, the size of the j-th sub-interval is:

(6).

The boundaries (connection points) of the sub-intervals are given with the set of data points

$$T = \left\{ t_j ;\ j = 1, 2, ..., K \right\} \qquad (7),$$

ki morajo izpolnjevati naslednje pogoje:

which must fulfill the following conditions:

$$3 \le K \le N \qquad (8)$$

$$t_1 = x_1 \ ;\ t_K = x_N \qquad (9)$$

$$l_j > 0; \quad j = 1, 2, ..., K-1 \qquad (10).$$

Točke t_j bomo imenovali vozlišča.

Points t_j are denoted as connection points.

1.2 Izpeljava algoritma ([1] do [3])

1.2 Outline of the algorithm ([1] to [3])

Znotraj vsakega koraka:

Within each of the sub-intervals:

$$I_j = \left[t_j, t_{j+1} \right]; \quad j = 1, 2, 3, ..., K-1$$

uporabimo polinom tretjega reda:

we utilize the third-order polynomial:

$$f_j(x) = A_j x^3 + B_j x^2 + C_j x + D_j \qquad (11),$$

ki naj na meji s sosednjima korakoma, tj., v j-tem in j+1 vozlišču, izpolnjuje naslednje pogoje:

which at the borders of the sub-interval, i.e., at the connection points j and j+1, fulfills the conditions:

$$f_j(t_j) = f_{j-1}(t_j) = F_j; \quad f_j(t_{j+1}) = f_{j+1}(t_{j+1}) = F_{j+1} \qquad (12)$$

$$f'_j(t_j) = f'_{j-1}(t_j) = P_j; \quad f'_j(t_{j+1}) = f'_{j+1}(t_{j+1}) = P_{j+1} \qquad (13)$$

$$f''_j(t_j) = f''_{j-1}(t_j) = H_j; \quad f''_j(t_{j+1}) = f''_{j+1}(t_{j+1}) = H_{j+1} \qquad (14).$$

Iz linearnosti drugega odvoda gladilne funkcije (sl. 1) izhaja:

From the linearity of the second derivative of the smoothing function, Fig. 1, follows:

$$\frac{t_{j+1} - x}{x - t_j} = \frac{H_{j+1} - f''_j(x)}{f''_j(x) - H_j} \qquad (15)$$

in od tod:

and

$$f''_j(x) = H_j \frac{t_{j+1} - x}{l_j} + H_{j+1} \frac{x - t_j}{l_j} \qquad (16).$$

Dvakratno integriranje enačbe (16) da:

Double integration of Eq. (16) yields:

$$f'_j(x) = -\frac{H_j}{2l_j}\left(t_{j+1} - x\right)^2 + \frac{H_{j+1}}{2l_j}\left(x - t_j\right)^2 + E_1 \qquad (17)$$

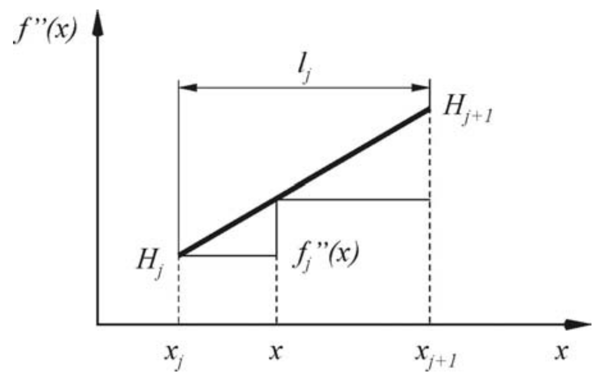
$$f_j(x) = \frac{H_j}{6l_j}\left(t_{j+1} - x\right)^3 + \frac{H_{j+1}}{6l_j}\left(x - t_j\right)^3 + E_1 x + E_2 \qquad (18),$$

kjer integracijski stalnici E_1 in E_2 določimo iz pogoja (12):

where the integration constants E_1 and E_2 can be obtained from the conditions (12):

$$E_1 = \frac{F_{j+1} - F_j}{l_j} - \frac{l_j\left(H_{j+1} - H_j\right)}{6} \qquad (19)$$

$$E_2 = t_{j+1}\left(\frac{F_j}{l_j} - \frac{l_j H_j}{6}\right) - t_j\left(\frac{F_{j+1}}{l_j} - \frac{l_j H_{j+1}}{6}\right) \qquad (20).$$



Sl. 1. *Drugi odvod približne funkcije znotraj j-tega koraka*
Fig. 1. *Second derivative of the approximation function inside the j-th sub-interval*

Iz razmerij (18) do (20) bi sedaj lahko izračunali stalnice A_j, B_j, C_j in D_j, definirane z enačbo (11). Iz praktičnih razlogov bomo stalnice polinoma ohranili izražene v odvisnosti od F_j, P_j, H_j in l_j (glej enačbe (12) do (14) in sliko1). Enačbi (17) in (18) sedaj lahko zapišemo kot:

The constants of the polynomials within each sub-interval, A_j, B_j, C_j and D_j, Eq. (11), can be calculated from the relations (18) through (20). For practical reasons the constants will be expressed in terms of F_j, P_j, H_j and l_j, (see Eqs. (12) to (14) – and Fig. 1). Equations (17) and (18) can now be rearranged as:

$$f_j'(x) = -H_j\left[\frac{(t_{j+1}-x)^2}{2l_j} - \frac{l_j}{6}\right] + H_{j+1}\left[\frac{(x-t_j)^2}{2l_j} - \frac{l_j}{6}\right] - \frac{F_j}{l_j} + \frac{F_{j+1}}{l_j} \quad (21)$$

$$f_j(x) = H_j\left[\frac{(t_{j+1}-x)^3}{6l_j} - l_j\frac{t_{j+1}-x}{6}\right] + H_{j+1}\left[\frac{(x-t_j)^3}{6l_j} - l_j\frac{x-t_j}{6}\right] + F_j\left[\frac{t_{j+1}-x}{l_j}\right] + F_{j+1}\left[\frac{x-t_j}{l_j}\right] \quad (22).$$

Iz pogoja (13) izhaja:

From the condition (13) it follows:

$$H_j\frac{l_j}{6} + H_{j+1}\left[\frac{l_j+l_{j+1}}{3}\right] + H_{j+2}\frac{l_{j+1}}{6} - \frac{F_j}{l_j} + F_{j+1}\left(\frac{1}{l_j}+\frac{1}{l_{j+1}}\right) - \frac{F_{j+2}}{l_{j+1}} = 0 \quad (23),$$

kjer je $j = 1, 2, ..., K–2$. Dobili smo sistem $K–2$ enačb z $2K$ neznankami, H_k in F_k, kjer je $k = 1, 2, ..., K$. Za enolično rešitev problema potrebujemo še dodatnih $K+2$ enačb.

where $j = 1, 2, ..., K–2$. We obtained the system of $K–2$ equations with $2K$ unknowns, i.e., H_k and F_k, where $k = 1, 2, ..., K$. Hence, in order to solve the problem, we need additional $K+2$ equations.

Določitev F_i

Determination of F_i

Naslednjih K dodatnih enačb lahko dobimo na dva načina:

a) V primeru, ko je število izbranih vozlišč enako številu podanih diskretnih točk, $K = N$ in $x = t_j$, se bodo vozlišča ujemala s podanimi diskretnimi vrednostmi. V tem primeru je:

There are two ways of obtaining the next K additional equations:

a) When the number of connection points is the same as the number of given data points, $K = N$ and $x = t_j$, then the connection points coincide with the given set of discrete values. Hence:

$$\{F_j = y_j; \quad j = 1, 2, \cdots, K\} \quad (24).$$

V tem primeru gre izračunana krivulja natanko skozi vse diskretne vrednosti, kar pomeni, da dobimo interpolacijsko krivuljo množice točk $\mathcal{F}$, podane z izrazom (1). Ta postopek pomeni poseben primer metode, opisane v nadaljevanju.

In this case the calculated curve goes exactly through all the discrete values, meaning that we obtain an interpolation curve for the set of discrete datum points $\mathcal{F}$, Eq. (1). This case is a special case of the method described below.

b) Drugi, splošnejši postopek imamo, ko je število izbranih vozlišč manjše od števila podanih diskretnih vrednosti, $K < N$. V tem primeru določimo funkcijske vrednosti v vozliščih $\{F_j; j = 1, 2, ..., K\}$ z metodo najmanjših kvadratov. Vozlišča $\{t_j; j = 1, 2, ..., K\}$ moramo izbrati tako, da bo vsak od korakov $\{l_j; j = 1, 2, ..., K\}$ vseboval vsaj en x_i.

V nadaljevanju bomo analizirali samo metodo b), ki je splošnejša.

Vsota kvadratov odstopkov med vrednostmi, izračunanimi iz gladilne funkcije, $f_j(x_i)$, in izmerjenimi diskretnimi vrednostmi y_i znotraj j-tega koraka, je:

b) We have a more general case when the number of selected connection points is smaller than the number of given discrete datum points, i.e., $K < N$. In this case the values at the connection points $\{F_j; j = 1, 2, ..., K\}$ are determined with the least-squares method. The set of connection points $\{t_j; j = 1, 2, ..., K\}$ should be selected such that each of the sub-intervals $\{l_j; j = 1, 2, ..., K\}$ includes at least one x_i.

Here we will discuss only case b), as it is more general.

The sum of the squares of the deviations between the values computed from the spline function, $f_j(x_i)$, and the measured discrete values y_i within the j-th sub-interval is:

$$s_j = \sum_{i=v_{j-1}+1}^{v_j} \left[f_j(x_i) - y_i \right]^2 \tag{25}$$

Pri tem je v_j števec zadnje točke v koraku v_j. Seštevanje prek vseh K–1 korakov da skupno napako približka:

Here v_j is the index of the last data point within the sub-interval v_j. Summation over all K–1 sub-intervals yields the sum of the approximation errors:

$$\mathcal{S} = \sum_{j=1}^{K-1} s_j = \sum_{j=1}^{K-1} \sum_{i=v_{j-1}+1}^{v_j} \left[f_j(x_i) - y_i \right]^2 \tag{26}$$

Z minimiziranjem skupne napake dobimo:

Minimizing the sum errors we obtain:

$$\frac{\partial \mathcal{S}}{\partial F_k} = 2 \sum_{j=1}^{K-1} \sum_{i=v_{j-1}+1}^{v_j} \left[f_j(x_i) - y_i \right] \frac{\partial f_j(x_i)}{\partial F_k} = 0 \tag{27}$$

$$\sum_{j=1}^{K-1} \sum_{i=v_{j-1}+1}^{v_j} f_j(x_i) \frac{\partial f_j(x_i)}{\partial F_k} = \sum_{j=1}^{K-1} \sum_{i=v_{j-1}+1}^{v_j} y_i \frac{\partial f_j(x_i)}{\partial F_k} \tag{28}$$

Za vsak F_k, kjer je $k = 1, 2, ..., K$, dobimo enačbo oblike (28), kar pomeni naslednjih K enačb. Parcialne odvode $\partial f_j(x_i) / \partial F_k$ izračunamo z odvajanjem enačbe (22):

For each F_k, where $k = 1, 2, ..., K$, an equation of the form of Eq. (28) is obtained. This yields the next K equations. The partial derivatives $\partial f_j(x_i) / \partial F_k$ can be obtained from the Eq. (22):

$$\frac{\partial f_j(x_i)}{\partial F_k} = \begin{cases} \dfrac{(t_{j+1} - x)}{l_j}; & \text{za/for} \quad k = j \\ \dfrac{(x - t_j)}{l_j}; & \text{za/for} \quad k = j+1 \\ 0; & \text{za/for} \quad j \neq k \neq j+1 \end{cases} \tag{29}$$

Z upoštevanjem razmerij (29) preide enačba (28) v obliko:

Using the relations (29), Eq. (28) can be rearranged as:

$$\sum_{i=v_{k-2}+1}^{v_{k-1}} f_{k-1}(x_i) \frac{x_i - t_{k-1}}{l_{k-1}} + \sum_{i=v_{k-1}+1}^{v_k} f_k(x_i) \frac{t_{k+1} - x_i}{l_k} = \sum_{i=v_{k-2}+1}^{v_{k-1}} y_i \frac{x_i - t_{k-1}}{l_{k-1}} + \sum_{i=v_{k-1}+1}^{v_k} y_i \frac{t_{k+1} - x_i}{l_k} \tag{30}$$

Če sedaj upoštevamo še enačbo (22), dobimo:

Utilizing Eq. (22) we obtain:

$$\begin{aligned} &\sum_{i=v_{k-2}+1}^{v_{k-1}} \left\{ H_{k-1} \left[\frac{(t_k - x_i)^3}{6 l_{k-1}} - l_{k-1} \frac{t_k - x_i}{6} \right] + H_k \left[\frac{(x_i - t_{k-1})^3}{6 l_{k-1}} - l_{k-1} \frac{x_i - t_{k-1}}{6} \right] + F_{k-1} \left[\frac{t_k - x_i}{l_{k-1}} \right] + F_k \left[\frac{x_i - t_{k-1}}{l_{k-1}} \right] \right\} \left(\frac{x_i - t_{k-1}}{l_{k-1}} \right) + \\ &+ \sum_{i=v_{k-1}+1}^{v_k} \left\{ H_k \left[\frac{(t_{k+1} - x_i)^3}{6 l_k} - l_k \frac{t_{k+1} - x_i}{6} \right] + H_{k+1} \left[\frac{(x_i - t_k)^3}{6 l_k} - l_k \frac{x_i - t_k}{6} \right] + F_k \left[\frac{t_{k+1} - x_i}{l_k} \right] + F_{k+1} \left[\frac{x_i - t_k}{l_k} \right] \right\} \left(\frac{t_{k+1} - x_i}{l_k} \right) = \\ &= \sum_{i=v_{k-2}+1}^{v_{k-1}} y_i \frac{x_i - t_{k-1}}{l_{k-1}} + \sum_{i=v_{k-1}+1}^{v_k} y_i \frac{t_{k+1} - x_i}{l_k} \end{aligned} \tag{31}$$

oziroma / or

$$\mathcal{A}H_{k-1}+\mathcal{B}H_k+\mathcal{C}H_{k+1}+\mathcal{D}F_{k-1}+\mathcal{E}F_k+\mathcal{G}F_{k+1}=\mathcal{H}_{k+1} \quad (32),$$

kjer so: / where:

$$\mathcal{A}_k=\sum_{i=v_{k-2}+1}^{v_{k-1}}\left[\frac{(t_k-x_i)^3}{6l_{k-1}}-l_{k-1}\frac{t_k-x_i}{6}\right]\left(\frac{x_i-t_{k-1}}{l_{k-1}}\right) \quad (33)$$

$$\mathcal{B}_k=\sum_{i=v_{k-2}+1}^{v_{k-1}}\left[\frac{(x_i-t_{k-1})^3}{6l_{k-1}}-l_{k-1}\frac{x_i-t_{k-1}}{6}\right]\left(\frac{x_i-t_{k-1}}{l_{k-1}}\right)+\sum_{i=v_{k-1}+1}^{v_k}\left[\frac{(t_{k+1}-x_i)^3}{6l_k}-l_k\frac{t_{k+1}-x_i}{6}\right]\left(\frac{t_{k+1}-x_i}{l_k}\right) \quad (34)$$

$$\mathcal{C}_k=\sum_{i=v_{k-1}+1}^{v_k}\left[\frac{(x_i-t_k)^3}{6l_k}-l_k\frac{x_i-t_k}{6}\right]\left(\frac{t_{k+1}-x_i}{l_k}\right) \quad (35)$$

$$\mathcal{D}_k=\sum_{i=v_{k-2}+1}^{v_{k-1}}\frac{(t_k-x_i)(x_i-t_{k-1})}{l_{k-1}^2} \quad (36)$$

$$\mathcal{E}_k=\sum_{i=v_{k-2}+1}^{v_{k-1}}\frac{(x_i-t_{k-1})^2}{l_{k-1}^2}+\sum_{i=v_{k-1}+1}^{v_k}\frac{(t_{k+1}-x_i)^2}{l_k^2} \quad (37)$$

$$\mathcal{G}_k=\sum_{i=v_{k-1}+1}^{v_k}\frac{(x_i-t_k)(t_{k+1}-x_i)}{l_k^2} \quad (38)$$

$$\mathcal{H}_k=\sum_{i=v_{k-2}+1}^{v_{k-1}}y_i\frac{x_i-t_{k-1}}{l_{k-1}}+\sum_{i=v_{k-1}+1}^{v_k}y_i\frac{t_{k+1}-x_i}{l_k} \quad (39).$$

Enačbi (23) in (31) pomenita skupaj (2K–2) enačb, kar pomeni, da manjkata še dve enačbi. Zadnji dve enačbi dobimo iz robnih pogojev.

Eqs. (23) and (31) together represent (2K–2) equations. Two more equations are needed. These are obtained from the boundary conditions.

1.3 Robni pogoji

1.3 Boundary Conditions

Manjkajoči enačbi dobimo iz zahteve o ukrivljenosti krivulje na obeh koncih množice $\mathcal{F}$, tj. H_1 in H_K, ki ju zapišemo kot linearni funkciji ukrivljenosti v sosednjih točkah t_2 in t_{K-1}:

The missing two equations can be obtained from the condition that the curvatures on both ends of the set $\mathcal{F}$, i.e., H_1 and H_K, can be expressed as linear functions of the curvatures at the two neighboring points t_2 in t_{K-1}. Hence:

$$H_1=\lambda_1H_2+\lambda_2 \quad (40)$$

$$H_K=\lambda_3H_{K-1}+\lambda_4 \quad (41).$$

Z izbiro stalnic λ_1 do λ_4 lahko prilagajamo ukrivljenost krivulje na obeh koncih. V primeru $\{\lambda_i = 0; i = 1, ..., 4\}$ bosta, recimo, oba konca krivulje ravna.

Največkrat seveda nimamo informacij o obnašanju podatkov $\mathcal{F}$, ki jih analiziramo, na robovih. V tem primeru se izkaže kot najprimernejše, da H_1 in H_K določimo z minimizacijo integrala kvadratov ukrivljenosti krivulje:

With the selection of the constants λ_1 to λ_4 the curvature of the function at both ends can be adjusted as required. For example, when $\{\lambda_i = 0; i = 1, ..., 4\}$ both ends of the curve will be straight.

Usually, we do not have information about the behavior of the analyzed data, $\mathcal{F}$, at both ends. In such a case it is most appropriate to determine H_1 and H_K by minimizing the integral of the squares of the curve's curvatures:

$$\{U\}_{\min}=\left\{\int_{t_1}^{t_k}\left[f''(x)\right]^2dx\right\}_{\min} \quad (42).$$

Z upoštevanjem razmerja (16) dobimo:

Using relation (16) we obtain:

$$U = \sum_{j=1}^{K-1} \int_{t_j}^{t_{j+1}} \left[H_j \frac{t_{j+1} - x}{l_j} + H_{j+1} \frac{x - t_j}{l_j} \right]^2 dx \tag{43}$$

in po integraciji

and after integration

$$U = \frac{1}{3} \sum_{j=1}^{K-1} \left(H_{j+1}^2 + H_j H_{j+1} + H_j^2 \right) l_j \tag{44}$$

Minimizacijski postopek izvedemo z odvajanjem funkcije U po H_1 in H_K:

The minimization of the function U is obtained through a derivation with respect to H_1 and H_K:

$$\frac{\partial U}{\partial H_1} = \frac{l_1 \left(H_2 + 2H_1 \right)}{3} = 0 \tag{45}$$

$$\frac{\partial U}{\partial H_K} = \frac{l_{K-1} \left(2H_K + H_{K-1} \right)}{3} = 0 \tag{46}$$

Iz (45) in (46) izhaja:

From (45) and (46) it follows that:

$$H_1 = -\frac{H_2}{2} \tag{47}$$

$$H_K = -\frac{H_{K-1}}{2} \tag{48}$$

V primeru, ko izberemo na abscisi (osi x) en sam korak, bo $K = 2$ in $H_1 = H_2 = 0$, kar pomeni, da bo v tem primeru izveden približek podatkov s premico. K temu problemu se bomo ponovno vrnili v razpravi.

Izraza (47) in (48) sta manjkajoči dve enačbi. Skupaj z enačbami, ki ju definirata izraza (23) in (31), imamo sedaj sistem $2K$ linearnih enačb z $2K$ neznankami:

When on the abscissa (x-axis) we select only one interval, then $K = 2$ and $H_1 = H_2 = 0$, which means that the data will be approximated by a straight line. We will address this problem again later in the discussion.

Expressions (47) and (48) represent the missing two equations. Together with the expressions (23) and (31) we have now a system of $2K$ linear equations with $2K$ unknowns:

$$H_k \frac{l_k}{6} + H_{k+1} \left[\frac{l_k + l_{k+1}}{3} \right] + H_{k+2} \frac{l_{k+1}}{6} - \frac{F_k}{l_k} + F_{k+1} \left(\frac{1}{l_k} + \frac{1}{l_{k+1}} \right) - \frac{F_{k+2}}{l_{k+1}} = 0 \ , \ k = 1, 2, \cdots, K-2 \tag{49}$$

$$\mathcal{A}_k H_{k-1} + \mathcal{B}_k H_k + \mathcal{C}_k H_{k+1} + \mathcal{D}_k F_{k-1} + \mathcal{E}_k F_k + \mathcal{G}_k F_{k+1} = \mathcal{H}_{k+1}, \quad k = 1, 2, \cdots, K \tag{50}$$

$$H_1 + \frac{H_2}{2} = 0 \tag{51}$$

$$H_K + \frac{H_{K-1}}{2} = 0 \tag{52}$$

Stalnice $\mathcal{A}_k$, $\mathcal{B}_k$, $\mathcal{C}_k$, $\mathcal{D}_k$, $\mathcal{E}_k$, $\mathcal{G}_k$ in $\mathcal{H}_k$ so podane z enačbami (33) do (39). Dobljeni sistem enačb (49) do (52) rešimo numerično z eno izmed znanih metod za reševanje sistemov linearnih enačb.

Rešitev sistema linearnih enačb so funkcijske vrednosti interpolacijske krivulje v vozliščih $\{F_j, t_j; j = 1, 2, ..., K\}$, ter vrednosti pripadajočih drugih odvodov $\{H_j, t_j; j = 1, 2, ..., K\}$. Poljubno število diskretnih vrednosti interpolacijske krivulje lahko sedaj izračunamo z enačbo (23). V primeru, da nas zanimajo tudi vrednosti prvega in drugega odvoda, lahko te izračunamo z enačbama (21) in (16).

The constants $\mathcal{A}_k$, $\mathcal{B}_k$, $\mathcal{C}_k$, $\mathcal{D}_k$, $\mathcal{E}_k$, $\mathcal{G}_k$ and $\mathcal{H}_k$ are given by Eqs. (33) to (39). The obtained system of Equations (49) to (52) can be solved numerically using one of the existing methods for solving systems of linear equations.

The solutions of the system of linear equation are the values of the interpolation curve at the connection points $\{F_j, t_j; j = 1, 2, ..., K\}$, and the corresponding second derivatives $\{H_j, t_j; j = 1, 2, ..., K\}$. Any number of discrete data along the interpolation curve can be calculated using Eq. (23). To determine the corresponding values of the first and second derivative, Eqs. (21) and (16) can be used.

2 RAZPRAVA

Uporabnost izpeljanega algoritma za glajenje diskretno podanih krivulj bomo prikazali na treh primerih. V prvih dveh primerih smo diskretne vrednosti ustvarjali iz analitično podanih krivulj. Uporabili smo preprosto trigonometrično funkcijo $y = 50 + 40\sin x$ in ustvarili dve množici „eksperimentalnih“ podatkov. Prva množica:

$$\{\mathbf{A}\} = \{0 \le x_i \le 10,\ y_i = 50 + 40\sin x;\ i = 1, 2, \cdots, 41\} \quad (53)$$

je znotraj natančnosti računalnika brez napake. Druga množica:

$$\{\mathbf{B}\} = \{0 \le x_i \le 10,\ y_i = 50 + 40\sin x - 4.5 + 9 \cdot RND;\ i = 1, 2, \cdots, 41\} \quad (54)$$

pa vsebuje z dodatnimi členi (–4,5+9*RND*), kjer je *RND* ime vira naključnih števil od 0 do 1, numerično ustvarjeno 10% naključno napako. Množici sta v obliki polne črte in kvadratkov prikazani na sliki 2. Ta primera bosta namenjena za prikaz vpliva izbranega števila korakov na natančnost glajenja diskretnih podatkov.

V tretjem primeru bomo uporabili “prave” eksperimentalne podatke za realno $J'(\omega)$ in imaginarno $J''(\omega)$ komponento dinamične funkcije lezenja, ki smo jih poprej uporabili v okviru študija obrnjenega problema pri karakterizaciji materialnih funkcij viskoelastičnih materialov ([4] do [7]). Ta analiza je zahtevala predhodno „glajenje“’ izmerjenih materialnih funkcij, kar je vodilo do nastanka tega prispevka. Eksperimentalni podatki obeh materialnih funkcij so prikazani na sliki 3.

2.1 Minimalno število korakov

Za določitev minimalnega števila korakov, oziroma minimalnega števila vozlišč, smo uporabili podatke $\{\mathbf{A}\}$, ki so brez napake. Diskretne vrednosti na gladilnih krivuljah, izračunanih za različno število korakov, smo primerjali z analitičnimi vrednostmi. Kakovost približka je bila ocenjena s povprečno relativno napako $\mathcal{N}$:

$$\mathcal{N} = \frac{1}{N}\sum_{i=1}^{N} \frac{\sqrt{\left(y_{i,apr} - y_{i,teor}\right)^2}}{y_{i,teor}} \quad (55).$$

Z N smo označili število diskretnih podatkov, uporabljenih v izračunu približne krivulje, z $y_{i,apr}$ diskretne vrednosti na približni krivulji in z $y_{i,teor}$ pripadajoče funkcijske vrednosti brez napake.

2 DISCUSSION

The power of the proposed algorithm will be demonstrated on three different sets of discrete data. In the first two cases we will use the synthetic discrete data generated from the analytical function $y = 50 + 40\sin x$. The first set of “experimental” data:

is within the accuracy of the computer without an error, while the second set:

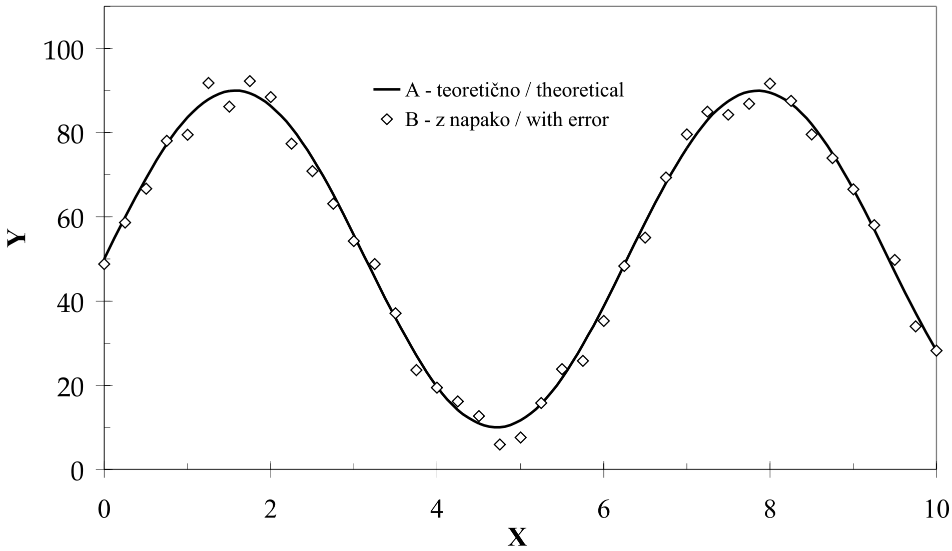
with the additional terms (–4.5+9*RND*), where *RND* represents a random generator of numbers between 0 and 1, incorporates a generated random 10% error. The two sets of data are shown in Fig. 2 as a solid line and diamonds, respectively. These two sets of data will be used to analyze the influence of the selected number of sub-intervals on the precision of smoothing discrete data.

In the third example we will use “true” experimental data on the real $J'(\omega)$ and the imaginary $J''(\omega)$ component of the creep-compliance function of poly-isobutylene. These data were used previously for studying inverse problems in the characterization of viscoelastic materials ([4] to [7]). In this analysis we had to smooth the data, which resulted in the paper presented here. Experimental data for both material functions are shown in Fig. 3.

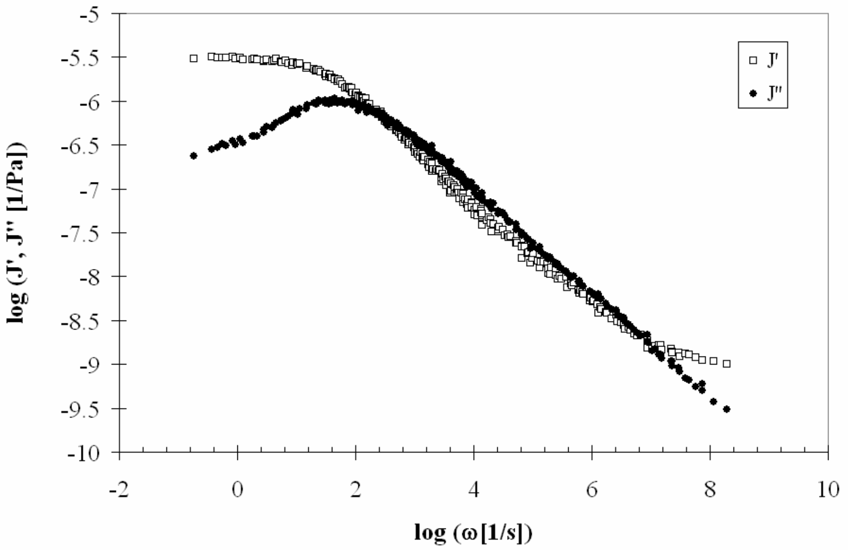
2.1. Minimum number of sub-intervals

To determine the minimum required number of sub-intervals we used the first set of discrete data, $\{\mathbf{A}\}$, which are within the resolving power of a computer without an error. Discrete values of the smoothing curve calculated for a different number of sub-intervals were compared with the corresponding analytical values. The accuracy of the approximation was evaluated with the average relative error, $\mathcal{N}$:

Here N denotes the number of discrete data used in the calculation of the approximation curve, $y_{i,apr}$ denotes the discrete values on the approximation curve, and $y_{i,teor}$ denotes the corresponding function-values without an error.



Sl. 2. *Ustvarjeni"eksperimentalni" podatki brez {**A**} in z naključno 10% napako {**B**}*
Fig. 2. *Generated "experimental" data without, {**A**}, and with a random 10% error, {**B**}*



Sl. 3. *Izmerjene diskretne vrednosti skupnih krivulj za realno, J'(ω), in imaginarno, J''(ω) komponento funkcije lezenja poli-izobutilena*
Fig. 3. *Measured discrete values of master curves for real, J'(ω), and imaginary, J''(ω), component of the creep compliance of poly-isobutylene*

Rezultat te analize je prikazan kot krivulja A v diagramu na sliki 4. Krivulja B je za podatke {**B**}, ki jih bomo analizirali pozneje. Zaradi boljše preglednosti je v notranjosti diagrama prikazan povečani del območja med 0 in 10% napake.

Primeri gladilnih krivulj izračunanih za različno število korakov, so prikazani na sliki 5. Zaradi preglednosti je prikazanih samo pet približnih krivulj, izračunanih za 1, 2, 3, 5 in 15 korakov.

The result of this analysis is shown as curve A in Fig. 4. Curve B shows the results for the set of data {**B**}, which will be discussed later. For reasons of clarity the enlarged segment of the curve between 0 and 10% of error is shown as an enclosure.

Examples of smoothing curves calculated for a different number of sub-intervals are shown in Fig. 5. For reasons of clarity we show only five approximation curves calculated for 1, 2, 3, 5 and 15 sub-intervals.

V primeru, ko izberemo en sam korak, bo približna krivulja premica. Ta lastnost krivulj zlepkov izhaja iz enačb (47) in (48). Ukrivljenosti na obeh koncih koraka sta namreč enaki nič, $H_1 = H_2 = 0$, kar pomeni, da je približna krivulja premica.

Če izberemo dva koraka, bosta ukrivljenosti gladilne krivulje na obeh koncih za polovico manjši od ukrivljenosti na stičišču obeh korakov, v skladu z enačbama (51) in (52). Gladilna krivulja bo v tem primeru parabolične oblike.

Sprejemljivo približno (gladilno) krivuljo dobimo šele pri petih korakih oziroma šestih vozliščih. Napaka približka je v tem primeru okrog 3,5%. S povečevanjem števila vozlišč se napaka približka hitro zmanjšuje, kakor to nazorno prikazuje krivulja A na sliki 4. Če izberemo 15 korakov, je relativna napaka že manjša od 0,2%. Z nadaljnjim povečevanjem števila vozlišč pridemo v mejni primer, ko je število vozlišč enako številu diskretnih podatkov. V tem primeru dobimo interpolacijsko krivuljo, ki povezuje vse točke. Ker so diskretni podatki {**A**} brez eksperimentalne napake, bo gladilna krivulja v bistvu enaka pripadajoči teoretični.

In the case when we choose only one sub-interval the approximation curve will be a straight line. This property of the spline curves results from the conditions (47) and (48). The curvatures at both ends of the sub-interval are equal to zero, i.e., $H_1 = H_2 = 0$, which means that the approximation curve is a straight line.

If we select two sub-intervals, the curvatures of the smoothing curve at both ends are half of the curvature in the connecting point of the two sub-intervals, in accordance with Equations (51) and (52). In this case, the shape of the smoothing curve will be parabolic.

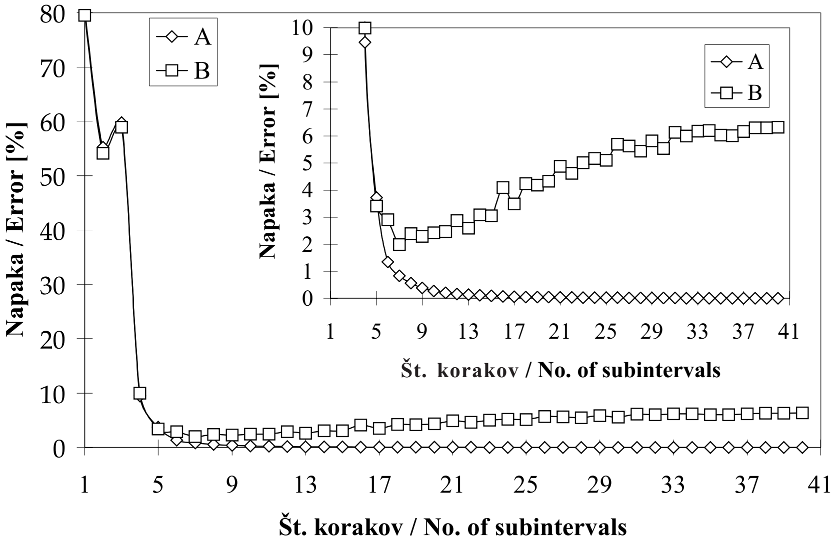
An acceptable approximation (smoothing) curve is obtained only after five sub-intervals, i.e., six connecting points. In this case the error of the approximation is about 4.5%. The error of the approximation will decrease with the increased number of sub-interval, as shown with the curve A in Fig. 4. If we choose 15 sub-intervals the relative error will be less than 0.2%. With a further increase in the number of sub-intervals we approach the limiting case when the number of connecting points is equal to the number of datum points. In such a case we obtain an interpolation curve, which connects all the datum points. Since the discrete data {**A**} are without experimental error, the smoothing curve will be essentially identical to the underlying theoretical curve.

2.2 Optimalno število korakov

Množica izmerjenih podatkov, ki jih želimo v praksi približati, vsebuje zmeraj določeno napako. V

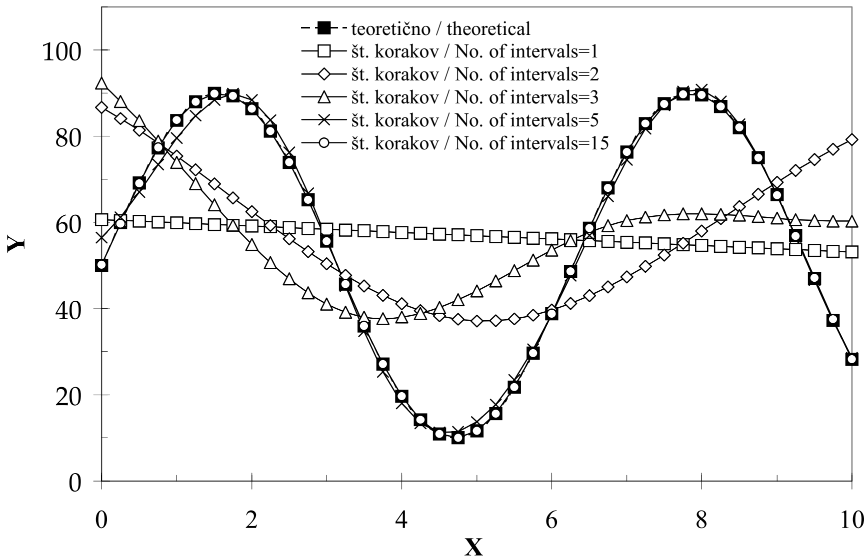
2.2 Optimum number of sub-intervals

Measured data, which we want to approximate, always contain some experimental error. In such cases



Sl. 4. *Napaka približka v odvisnosti od števila korakov, A – za približek krivulje brez naključne napake, B – približek krivulje z ±10% naključno napako*

Fig. 4. *Error of the approximation as a function of the number of sub-intervals, A – for the approximation of the theoretical curve, B – for the approximation of the curve with the added ±10% random error*



Sl. 5. *Približne krivulje z različnim številom korakov*
Fig. 5. *Approximation curves with a different number of sub-intervals*

teh primerih uporabimo gladilne funkcije za določitev gladkih približnih krivulj. Število korakov mora biti torej manjše od števila diskretnih podatkov. Sedaj stojimo pred pomembnim vprašanjem: Kolikšno je optimalno število korakov?

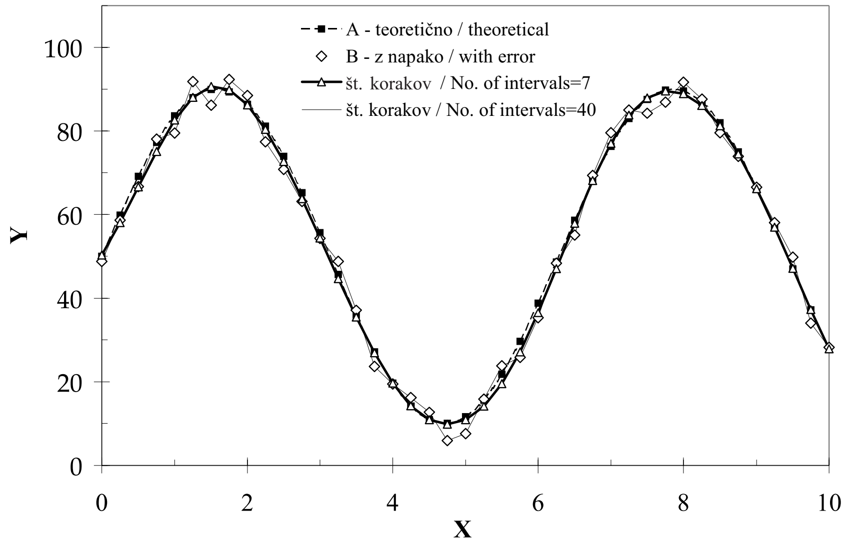
Da bi dobili odgovor na to vprašanje, smo uporabili množico podatkov {**B**}, enačba (54), ki vsebujejo naključno 10-odstotno napako. Diskretne vrednosti so v obliki kvadratkov prikazane na sliki 2. Podobno kakor v prejšnjem primeru, smo tudi tokrat napako glajenja ocenjevali v skladu z enačbo (55), tj. vrednosti dobljene z glajenjem smo primerjali s teoretičnimi funkcijskimi vrednostni, ki ne vsebujejo napake. Rezultat te analize je prikazan na sliki 4 kot krivulja B. Iz diagrama je razvidno, da je napaka približka v primeru, ko je število korakov enako ali manjše od 5, praktično enaka kakor v primeru, če podatki ne vsebujejo „eksperimentalne“ napake. S povečevanjem števila korakov se bo napaka najprej zmanjšala, nato pa se bo ponovno začela zvečevati. V trenutku, ko je število vozlišč enako številu diskretnih podatkov (krivulja gre v tem primeru natančno skozi vse diskretne vrednosti), bo napaka približka enaka povprečni eksperimentalni napaki, ki jo vsebuje množica diskretnih vrednosti {**B**}, v tem primeru približno 6 odstotkov.

S slike 4 je razvidno, da bomo dobili najboljši rezultat glajenja podatkov {**B**}, če izberemo 7 korakov. Na sliki 6 je ta primer približka prikazan v obliki trikotnikov, povezanih s polno črto. V istem diagramu je s polno črto prikazan tudi približek s 40

we use spline functions to obtain smooth continuous curves. Therefore, the number of selected sub-intervals should be smaller than the number of datum points. This raises an important question: What is the optimum number of sub-intervals?

To answer this question we have used the set of data {**B**}, Eq. (54), with a 10% random error. The data are shown as diamonds in Fig. 2. As in the previous case the quality of the smoothing was evaluated according to Eq. (55), i.e., discrete values predicted with the spline function were compared to the underlying theoretical values. The result of this analysis is presented in Fig. 4 as curve B. From the diagram it is clear that the error of splining the data with a 10% random error is about the same as for the data with no “experimental” error, if the selected number of sub-intervals is equal to or less than five. If we increase the number of sub-intervals the error of smoothing will first decrease and then start to increase again. We reach the limiting case when the number of connecting points is the same as the number of datum points. In this case the smoothing curve goes through all the datum pints, and the error of the approximation becomes equal to the average relative error of the set of data, {**B**}, which in this case is approximately 6%.

As seen from Fig. 4 we will get the best smoothing of the set of data {**B**} if we choose six sub-intervals. The result of this smoothing is shown in Fig. 6 as a line with triangles. In the same figure the approximation with 40 sub-intervals, i.e., 41 connecting points, is also shown as a solid line. In this case the



Sl. 6. *Približek funkcije, podane z 10-odstotno napako*
Fig. 6. *Approximation of function given with a 10% error*

koraki oziroma 41 vozlišči. V tem primeru gladilna krivulja povezuje diskretne vrednosti, kar pomeni, da v resnici glajenja ni.

Znotraj posameznega koraka je povprečna relativna napake približka odvisna od števila diskretnih vrednosti v tem koraku. Diagram na sliki 7 prikazuje takšno analizo za primer glajenja podatkov {**B**} z 10 koraki. Velikost napake glajenja se zmanjšuje s povečanim številom podatkov znotraj koraka in se stabilizira pri približno 30 podatkih na korak, kar se ujema s tistim, kar vemo iz statistike. Nadaljnje povečevanje števila točk na korak bistveno ne bo prispevalo h kakovosti glajenja.

2.3 Glajenje viskoelastičnih materialnih odvisnosti

Kot zadnji primer si oglejmo sedaj še uporabo predstavljenega algoritma na eksperimentalnih podatkih za realno, $J'(\omega)$, in imaginarno, $J''(\omega)$, komponento funkcije lezenja za nezamrežen poliizobutilen. Te eksperimentalne podatke smo pred tem analizirali v okviru študija obrnjenega problema pri analizi viskoelastičnih materialnih funkcij [6]. Podatki so bili povzeti iz [8], kjer so v pregledničniobliki podani odseki krivulj za različne temperaturne razmere. Na podlagi časovno-temperaturnega superpozicijskega načela smo konstruirali skupni krivulji za temperaturo T = 20 °C, po postopku, ki je opisan v [6]. Skupni krivulji sta predstavljeni v obliki polnih krogcev in kvadratkov na sliki 3.

Krivulji, ki ju dobimo z interpolacijo z uporabo gladilne funkcije, sta predstavljeni v obliki polne črte

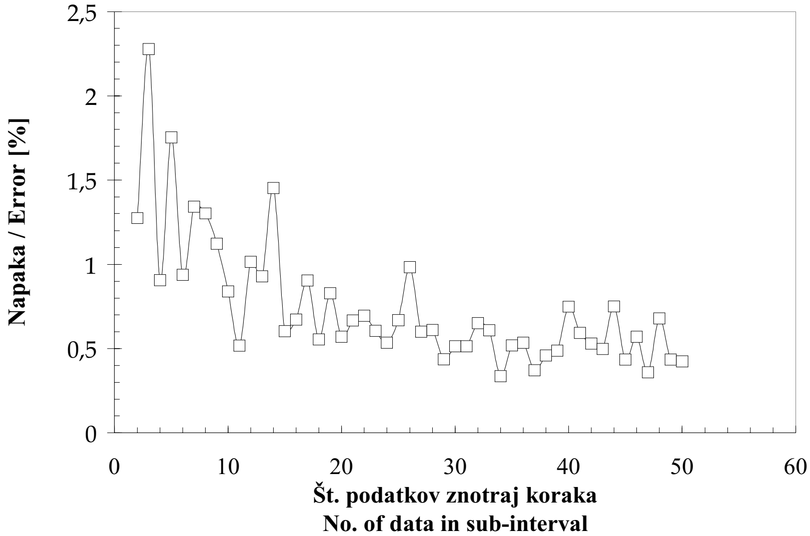
smoothing curve connects the discrete values, which essentially means that there is no smoothing.

The average relative error of smoothing depends on the number of datum points within each sub-interval. Figure 7 shows such an analysis for the case of smoothing the set of data {**B**} with 10 sub-intervals. The error of smoothing decreases with the number of datum points per sub-interval, and it stabilizes at about 30 datum points per sub-interval, which is in agreement with what we know from the statistics. Further increasing the number of datum points per sub-interval will not lead to substantially improved smoothing.

2.3 Smoothing of the viscoelastic material functions

The final demonstration of the power of the presented algorithm will be executed on the experimental data on the real, $J'(\omega)$, and the imaginary, $J''(\omega)$, components of the creep-compliance function of an uncrosslinked poly-isobutylene. We have used these data before [6] for studying the inverse problem of viscoelastic materials functions. The experimental data were taken from [8], where they are given in a tabular form as segments of the creep curve measured at different temperatures. Using the time-temperature superposition principle we have constructed the master curves for the reference temperature T = 20°C, as described in [6], which are shown as filled circles and squares in Fig. 3.

The two curves obtained after the smoothing with spline functions are shown in Fig. 8 as solid lines.



Sl. 7. *Napaka približka v odvisnosti od števila podatkov znotraj koraka*
Fig. 7. *Error of the approximation as a function of the number of datum points per sub-interval*

na sliki 8. Glajenje je bilo izvedeno z 10 koraki. Z gladilno funkcijo lahko preberemo poljubno število diskretnih vrednosti, kar je pomembno za nadaljnjo numerično analizo izmerjenih podatkov, posebno v primeru reševanja obrnjenih problemov. V tem primeru smo izračunali 10 diskretnih vrednosti na dekado vzdolž logaritemske frekvenčne koordinate.

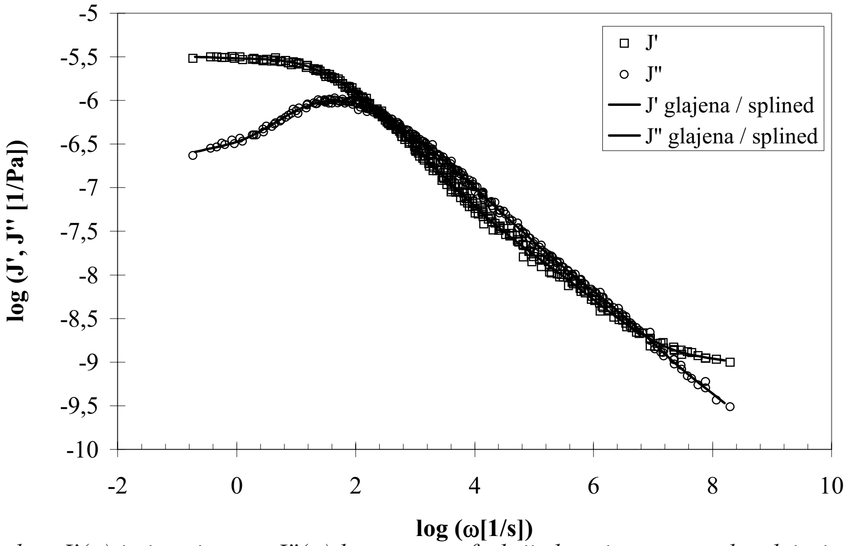
The smoothing procedure was executed with 10 sub-intervals. Using spline functions one can calculate as many discrete datum points as necessary, which is very important for any further numerical analysis of the experimental data, in particular for solving the inverse problems. In this case we have calculated 10 values per-decade along the logarithmic frequency axis.

3 SKLEP

Na temelju izvedene analize lahko ugotovimo, da ni enoličnega odgovora na vprašanje: "Katero

3 CONCLUSION

From the presented analysis we can conclude that there is no unique answer to the question: "What



Sl. 8. *Realna, J'(ω) in imaginarna, J''(ω) komponenta funkcije lezenja po postopku glajenja z gladilno funkcijo*
Fig. 8. *The real, J'(ω), and the imaginary, J''(ω), component of the creep compliance function after smoothing with the spline functions*

število korakov moramo izbrati za optimalno glajenje diskretnih podatkov?" Izbira števila korakov je in zmeraj bo "stvar osebne odločitve uporabnika". To si velja še posebej zapomniti v primerih, ko uporabljamo tržne programe, pri katerih nimamo vpogleda v algoritem uporabljen za glajenja diskretnih podatkov. V določenih primerih lahko tak postopek glajenja vodi tudi do neustrezne razlage meritev [9].

number of subintervals should be selected for optimum smoothing of discrete data?" Selection of the number of sub-intervals is, and will always be, a "personal decision by the user". This should be remembered when we are using commercial software packages where we have no information on the algorithm used for the process of smoothing discrete data. In some cases, such an approach may lead to an inappropriate interpretation of measurements [9].

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