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ABSTRACT

We propose several one-pass methods for data fitting in which a piecewise polynomial is used as an approximating function. The polynomial pieces are calculated step-by-step by the method of least squares as the data is scanned only once from the beginning to the end. To calculate the least squares fitting in each step, we use three classes of data, namely: the data in the current interval for which we want to determine the approximation, the data on the right side of this interval, and the data on the left side of this interval. The stability of the proposed algorithms is analyzed, and it is shown that a stable algorithm is obtained for all the one-pass methods proposed here.

1. INTRODUCTION

Recently, laboratory automation has become important, since microcomputers can now be used conveniently for on-line processing of measurement data. By using a microcomputer, we can make an automatic processing system of measurement data inexpensively.

For on-line processing of measurement data, it is useful to fit the data step-by-step from the beginning. In this case, least squares approximation by a single-pass method is good, because such an approximation is flexible, requires little computation time and small memory. Furthermore the approximation is obtained with little time lag to the data used.

A basic idea of one-pass method was proposed by Rice [1], and after that it was studied further by Ichida, Yoshimoto and Kiyono [2, 3]. However, the study by Ichida et al. was restricted to the case of piecewise cubic polynomials. Here, in order to search for the best method, we study one-pass methods with piecewise polynomials whose degree is not only three but two and four. We propose several kinds of one-pass methods and analyze the stability of the proposed methods.

2. LEAST SQUARES FITTING BY ONE-PASS METHODS

Suppose we have the data expressed by

$$F_k = f(x_k) + \epsilon_k \quad (k = 1, 2, \cdots), \tag{1}$$

where $f(x)$ is an unknown smooth function (signal), ϵ_k is an error having a mean of zero and variance σ^2 (less than ∞), and x_k is a sample point. We wish to fit a piecewise polynomial to the data step-by-step from the beginning to the end.

The methods presented here are grouped in two types, namely: Method A and Method B. Method A is shown in Fig. 1. We proceed fitting from left to right, and currently we wish to fit an approximating function for the interval I. In Fig. 1, s is a knot already determined, and y_0, m_0 and M_0 mean the function value, the value of the first derivative and the value of the second derivative at the knot s, respectively. Moreover, t is a knot we currently wish to determine from the data. The meaning of y, m and M is similar to the meaning of y_0, m_0 and M_0.

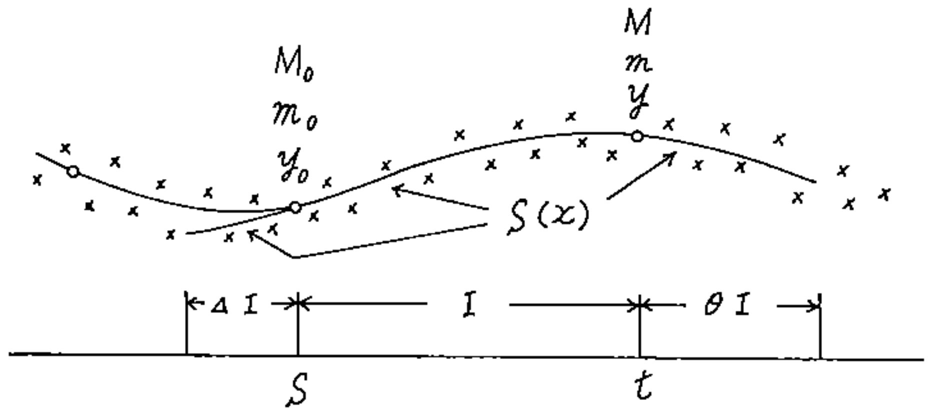

Fig. 1 Least squares fitting with Method A.

We determine an approximating function $S(x)$ by the method of least squares. For the sum of the squares of the residuals we use the data not only in the interval I but also in the intervals ΔI and θI, where the data in ΔI are called "past data" and the data in θI are called "future data". The approximating function $S(x)$ is used for the calculation of the least squares fitting for the intervals ΔI, I and θI. However, the approximation for the intervals ΔI and θI is only tentatively computed to get a smooth approximation in the interval I. Then, the sum of the squares of the residuals is expressed by

$$Q_A = \sum_{x_k \in \Delta I + I + \theta I} \{S(x_k) - F_k\}^2. \tag{2}$$

Fig. 2 shows Method B. We use a function $R(x)$ to approximate tentatively the data in the interval θI, where the functions $R(x)$ and $S(x)$ are joined with each other at the knot t with the same continuity condition at the knot s. We do not use function $S(x)$ for the interval θI. This is different from Method A. We determine an approximating function $S(x)$ by the method of least squares as in Method A. However, for the sum of the squares of the residuals in Method B we use

$$\begin{aligned} Q_B = &\sum_{x_k \in \Delta I + I} \{S(x_k) - F_k\}^2 \\ &+ w \sum_{x_k \in \Delta \theta I + \theta I} \{R(x_k) - F_k\}^2, \end{aligned} \tag{3}$$

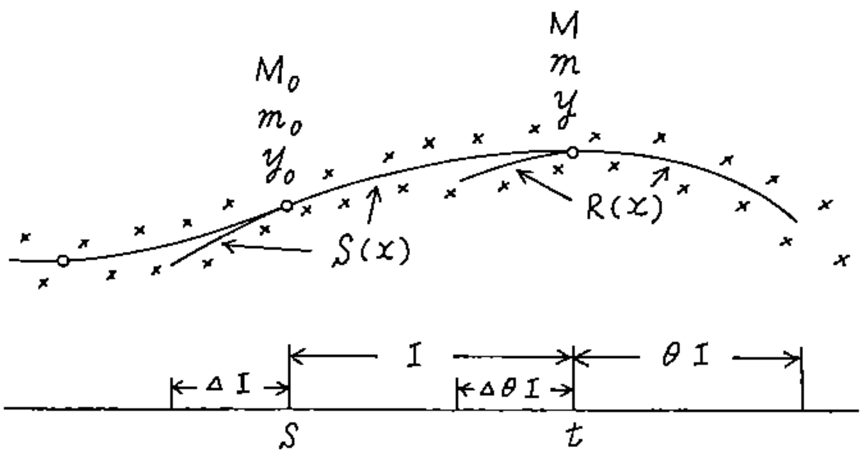

Fig. 2 Least squares fitting with Method B.

where w means a weighting factor for the second term.

We can construct several expressions of approximating functions applicable for the one-pass method. The amount of computation depends on the expressions. Thus, for the actual application we should choose the best one from the viewpoint of the amount of computation. However, here we use an expression with the function values and the values of the derivatives at the ends of polynomial pieces, because this expression is suitable for the analysis of stability.

For example, a cubic polynomial piece $S(x)$ which is continuous up to the second derivative at the knot s is expressed as

$$S(x)=y_0+m_0(x-s)+\frac{1}{2}M_0(x-s)^2+a(x-s)^3$$
$$\equiv S_{3,2}(x), \tag{4}$$

where a is a parameter to be determined by the method of least squares. We rewrite $S(x)$ to $S_{3,2}(x)$, where the subindex 3 means the degree of the polynomial piece and the subindex 2 means the continuity condition at the knot s. Similarly, a cubic polynomial piece $R(x)$ which is continuous up to the second derivative at the knot t is expressed as

$$R(x) = y + m(x-t) + \frac{1}{2}M(x-t)^2 + b(x-t)^3$$
$$= R_{3,2}(x), \tag{5}$$

where b is a parameter to be determined by the method of least squares. In the same way as the function $S(x)$, we rewrite $R(x)$ to $R_{3,2}(x)$.

Note that we can eliminate y, m and M by the following continuity condition at the knot t,

$$\left.\begin{aligned} y &= y_0 + m_0 h + \frac{1}{2}M_0 h^2 + a h^3 \\ m &= m_0 + M_0 h + 3ah^2 \\ M &= M_0 + 6ah \end{aligned}\right\}, \tag{6}$$

where $h = t - s$.

The first equation in eq. (6) shows the continuity of the value of the piecewise polynomial. Similarly, the second equation shows the continuity of the first derivative and the third equation shows the continuity of the second derivative.

Since the higher the degree of a piecewise polynomial the bigger the amount of computation will be, it is preferable to use a piecewise polynomial of as low degree as possible. On the other hand, if we wish to obtain a smooth approximation we should use a piecewise polynomial of as high degree as possible. According to the tradeoff between the two needs, it seems that the degrees of piecewise polynomials for good one-pass methods are within the range from second to forth. Thus, we concentrate our study in this case. Then, the approximating functions are grouped in Table 1; that is, the methods A and B are both subgrouped in four cases: A-1 to A-4 and B-1 to B-4.

3. STABILITY ANALYSIS OF THE ALGORITHM

A key point that makes a one-pass method feasible is the stability of algorithm. Therefore we should study, before constructing actual software for the one-pass methods, whether or not the methods we propose are stable. Figs. 3 and 4 show

Table 1 Grouping of the approximating functions.

Name of methods		Degree	Continuity condition	Approximating function $S(x)$	Approximating function $R(x)$
A	A-1	2	C^1	$S_{2,1}(x)$	
	A-2	3	C^1	$S_{3,1}(x)$	
	A-3	3	C^2	$S_{3,2}(x)$	
	A-4	4	C^2	$S_{4,2}(x)$	
B	B-1	2	C^1	$S_{2,1}(x)$	$R_{2,1}(x)$
	B-2	3	C^1	$S_{3,1}(x)$	$R_{3,1}(x)$
	B-3	3	C^2	$S_{3,2}(x)$	$R_{3,2}(x)$
	B-4	4	C^2	$S_{4,2}(x)$	$R_{4,2}(x)$

results of fitting by using one-pass methods. Fig. 3 is a case where the algorithm is stable and a good result is obtained. Fig. 4 is a case where the algorithm is unstable and a bad result is obtained.

The problem of the stability is solved as follows. First, in Method A we determine the parameters of the approximating function $S(x)$ by using the condition that eq. (2) is minimized. Similarly, in Method B we determine the parameters of the approximating functions $S(x)$ and $R(x)$ by using the condition that eq. (3) is minimized. Second, we substitute these parameters to an equation of the continuity condition at the knot t. Then, we get a difference equation among y_0, m_0, y and m for the approximation of class C^1 or a difference equation among y_0, m_0, M_0, y, m and M for the approximation of class C^2. Third, we examine the stability of the

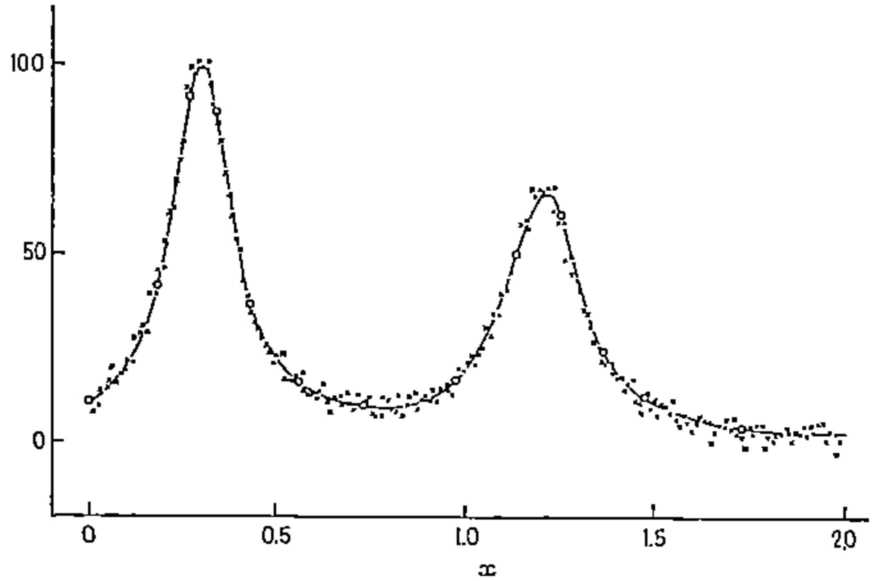

Fig. 3 Result of fitting by using a stable algorithm [3].

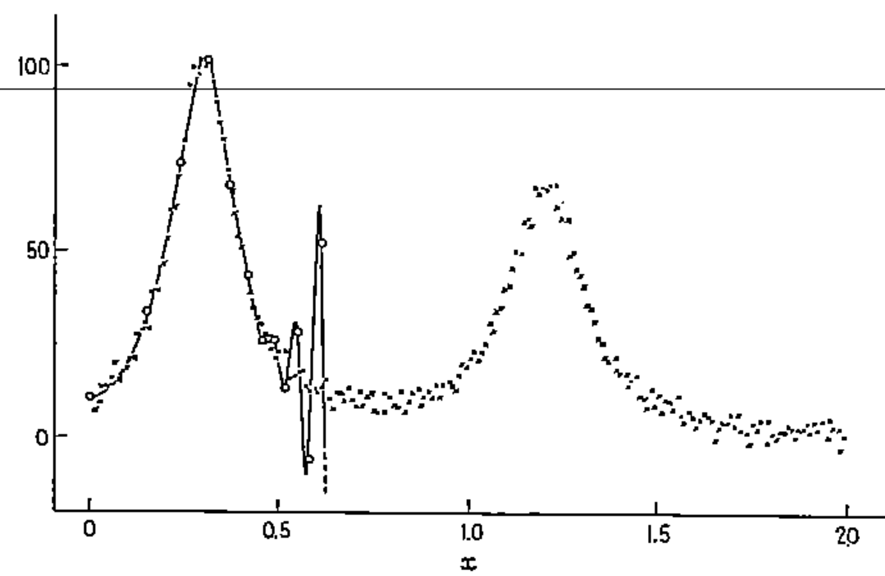

Fig. 4 Result of fitting by using an unstable algorithm [3].

difference equations.

However, if we use these difference equations for stability analysis, the analysis becomes very difficult, because derivation of the equations is not easy and moreover the equations have variable coefficients in general. Thus, we introduce two kinds of idealizations. The first is that the sampling intervals of data are equal and short enough so that the summation can be replaced by an integral. Then, the sum of the squares of the residuals for the Method A (eq. (2)) becomes

$$Q_A = \int_{s-\Delta I}^{t+\theta I} \{S(x) - F(x)\}^2 dx, \tag{7}$$

and the sum of the squares of the residuals for the Method B (eq. (3)) becomes

$$\begin{aligned} Q_B &= \int_{s-\Delta I}^{t} \{S(x) - F(x)\}^2 dx \\ &+ w \int_{t-\Delta\theta I}^{t+\theta I} \{R(x) - F(x)\}^2 dx. \end{aligned} \tag{8}$$

In Method A, we determine the parameters of the approximating function $S(x)$ by using the condition that eq. (7) is minimized. Similarly, in Method B we determine the parameters of the approximating function $S(x)$ and $R(x)$ by using the condition that eq. (8) is minimized. Substituting these parameters to the equation of the continuity condition at the knot t, we obtain the following difference equations,

$$\begin{bmatrix} y \\ m \end{bmatrix} = \begin{bmatrix} d_{11} & d_{12}h \\ d_{21}h^{-1} & d_{22} \end{bmatrix} \begin{bmatrix} y_0 \\ m_0 \end{bmatrix} + \begin{bmatrix} e_1 \\ e_2 \end{bmatrix} \tag{9}$$

for the approximation of class C^1 and

$$\begin{bmatrix} y \\ m \\ M \end{bmatrix} = \begin{bmatrix} d_{11} & d_{12}h & d_{13}h^2 \\ d_{21}h^{-1} & d_{22} & d_{23}h \\ d_{31}h^{-2} & d_{32}h^{-1} & d_{33} \end{bmatrix} \begin{bmatrix} y_0 \\ m_0 \\ M_0 \end{bmatrix} + \begin{bmatrix} e_1 \\ e_2 \\ e_3 \end{bmatrix} \tag{10}$$

for the approximation of class C^2. Here the d's are constants which depend on θ, Δ and w but not on h. Let us recall that h is the length of the interval I. Moreover, the e's are not constants and depend on the function $F(x)$, but they do not depend on y_0, m_0, M_0, y, m and M.

These equations have variable coefficients in general, because h is different in each interval. Thus, we introduce the second idealization; that is, the intervals of the knots are equal. In this case, the coefficients of the difference equations become constants, and the stability is easily examined by the use of the eigenvalues for the coefficient matrices.

Figs. 5-9 show results of the maximum of the absolute values of the eigenvalues calculated in terms of some parameters. These parameters are θ (proportion of the number of the right side data), Δ (proportion of the number of the left side data), and w (weighting factor for the sum of the squares of the residuals for the right side data).

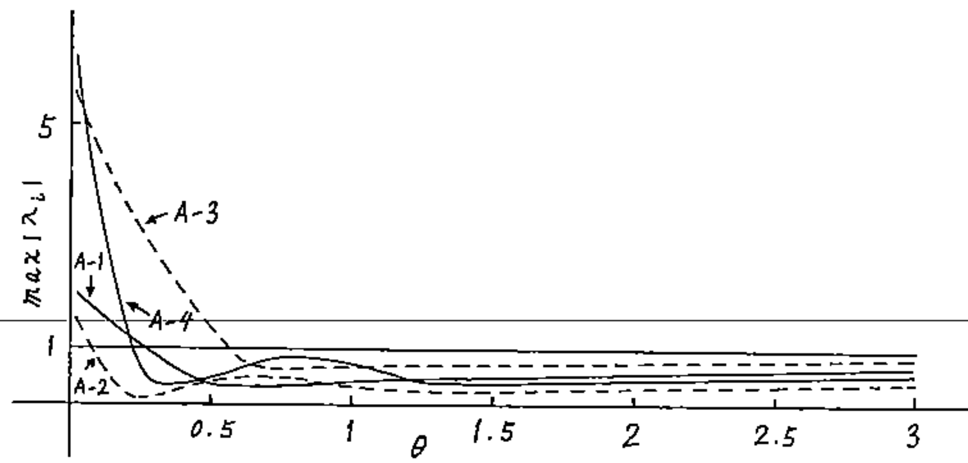

Fig. 5 The maximum of the absolute values of the eigenvalues of the coefficient matrices for the Method A ($\Delta = 0$).

Fig. 5 shows a result for the Method A. The abscissa θ means the relative amount of future data, and the ordinate, maximum of the $|\lambda_i|$, means the maximum of the absolute values of the eigenvalues. According to the theory of stability, a linear system is stable where the maximum of the $|\lambda_i|$ is less than one. Thus, Fig. 5 shows that the Method A is unstable when we use a small amount of future data. However, if we increase the amount of future data, the method becomes stable; the situation is fairly different among the methods A-1 to A-4. Here, let us recall that A-1 uses a piecewise quadratic polynomial, A-2 and A-3 use a piecewise cubic polynomial and A-4 uses a piecewise biquadratic polynomial. This figure corresponds to the case that Δ is equal to zero.

Fig. 6 shows the result for the case that $\Delta = 0.5$; that is, the amount of the past data is half the data in the current interval. The result is not so different from Fig. 5.

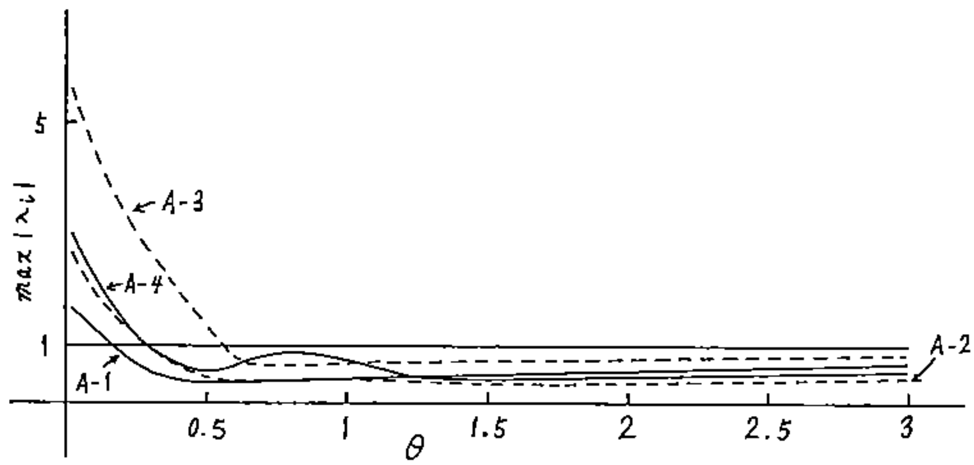

Fig. 6 The maximum of the absolute values of the eigenvalues of the coefficient matrices for Method A ($\Delta = 0.5$).

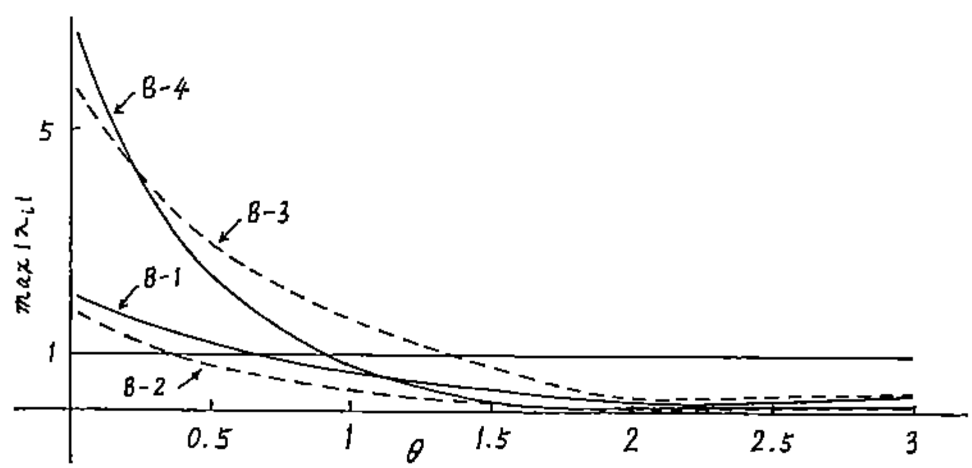

Fig. 7 The maximum of the absolute values of the eigenvalues of the coefficient matrices for Method B ($\Delta = 0$, $w = 1$).

A result of the Method B is shown in Fig. 7. The result is similar to the results of the Method A. However, in order to be stable, the Method B needs more future data than the Method A. Here, let us recall that B-1 uses a piecewise quadratic polynomial , B-2 and B-3 use a piecewise cubic polynomial and B-4 uses a piecewise biquadratic polynomial. Fig. 7 corresponds to the case that $\Delta = 0$ and $w = 1$.

Fig. 8 is a result for the case that $\Delta = 0.5$ and $w = 1$. We also get a stable algorithm in this case if we use enough of the future data.

Fig. 9 shows the relation between the stability and the weighting factor w for the case that $\Delta = 0.5$ in Method B-2. To stabilize the algorithm, the bigger the weighting factor, the smaller the amount of future data will be.

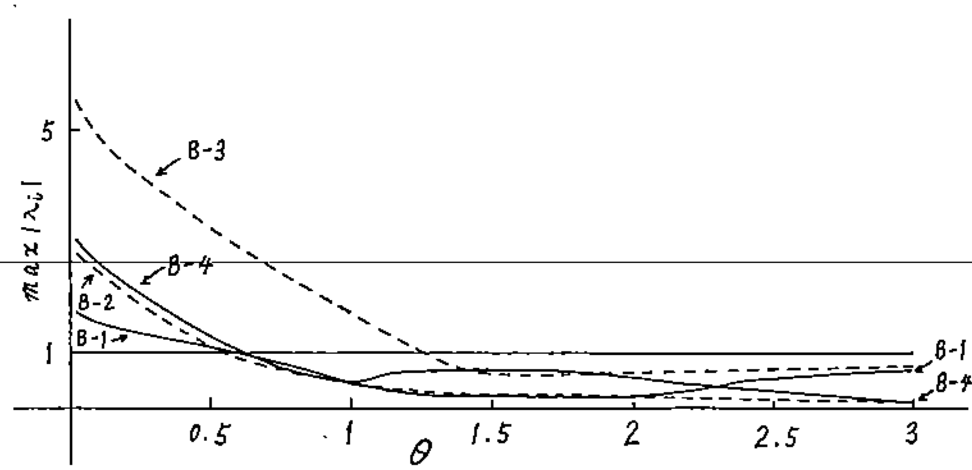

Fig. 8 The maximum of the absolute values of the eigenvalues of the coefficient matrices for Method B ($\Delta = 0.5$, $w = 1$).

In consequence of the analysis above, it is clear that we can get a stable algorithm in all the cases proposed here provided we use enough of the right side data (future data). However, the stability is strongly affected by the number of the right side data and by the weighting factor.

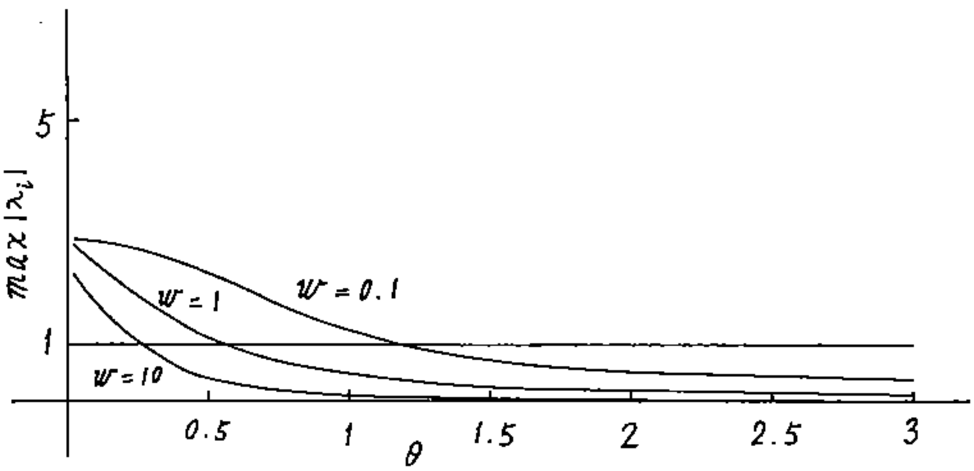

Fig. 9 The maximum of the absolute values of the eigenvalues of the coefficient matrices for Method B-2 ($\Delta = 0.5$).

4. CONCLUSION

We proposed several kinds of one-pass methods for data fitting in which a piecewise polynomial is used as an approximating function. The stability of the proposed methods is analyzed, and it is shown that a stable algorithm is obtained in all the cases proposed here. The evaluation of the performance of the proposed algorithms is an important open problem.

5. ACKNOWLEDGMENT

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