A Generalised Linear and Nonlinear Spline filter

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Received Date Line (to be inserted by Production) (8 pt)

Abstract

In this paper, a generalised spline filter, that has a unified description for both the linear spline filter and the nonlinear robust spline filter, is proposed. Based on the M-estimation theory, the general spline filter model can be solved by using an Iterated Reweighted Least Squared method which is also general for both the linear and nonlinear spline filter. The algorithm has been verified to be effective, efficient and fast.

Keywords: Generalised Spline filter, Robust filter, Nonlinear filter, M-estimation, Surface characterisation

1. Introduction

Filtration has always been important in surface metrology: it is the means by which the surface features of interest are extracted from the measured data for further analysis. Filtering techniques can help: (1)Judge whether the manufacturing process or manufacturing conditions are effective or out of control, whether specific events in the manufacturing processes have occurred; (2)Interpret functional properties of macro, micro and nano geometry, which reflect product properties, such as optical quality, tribological properties, service life, safety, reliability, etc [1].

The Gaussian filter is the most widely used standard filtering technique for surface characterisation. However, the following shortcomings have hampered its practical application in industry including: (1) the measured profile is truncated due to the boundary effect, especially when the measured data is not much longer than the cutoff wavelength; (2) it is unsuitable for surfaces with relatively large form components; and (3) it is unable to handle measurement outliers or residual profiles with non-Gaussian distributions.

Currently, there are two ways to solve the above problems. One is by using improved Gaussian regression filters, the other way is by using spline filters. To address the boundary effect and form removal issues with the traditional Gaussian filtering, Brinkman et al [2] have proposed a Gaussian regression filtering technique with the extension of up to second order polynomial form. By introducing a weighted iteration procedure, the Gaussian regression filter can obtain robust results against outliers [3]. A fast algorithm of the higher order nonlinear Gaussian regression filter was introduced recently[4]. The linear spline filter was proposed by Krystek [5] as a complementary method for the standard Gaussian filter. Compared with the standard Gaussian filter, it has the advantages of no boundary effect and follows the form well. ISO/TC213 has drafted a L1-norm based nonlinear

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procedure [6] to make the spline filter robust and Goto in Japan has reported a robust spline filter based on L2-norm [7]. However, both of these robust spline filters are confidential and there are no robust spline filter solutions and associated algorithms publicly available.

In this paper, a generalised spline filter based on spline theory and M-estimation theory is proposed. It makes the linear spline filter and the nonlinear robust filter have the same theoretical framework and can be deduced directly by choosing different error metrics in the general model. Section 2 gives the model of the generalised spline filter, and its solution is provided in section 3. Section 4 gives the detailed solution when using different estimators, and experimental results and discussions are shown in section 5. Finally, section 6 gives the conclusions.

2. Generalised Spline filter

The ordinary spline filter $s(x_k)$ can be described as follows: Let the data points $(x_i, z_i), (i = 0 \cdots n-1)$ be given, and assume them to be sorted in a strictly ascending order by the pivot points x_i, which are equidistant, and of width Δx, i.e. $x_0 < x_1 < \ldots x_{n-2} < x_{n-1}$ is valid. To find $s(x_k)$ the residual errors are minimized using the L2-norm together with the condition of minimizing the bending energy, which is proportional to $\int \left(\frac{d^2 s(x)}{dx^2} \right)^2 dx$, and the condition of natural boundary condition. According to the well known method of variational calculus, the spline filter $s(x_k)$ can be described as the following minimization problem [4,5]:

$$\sum_{k=0}^{n-1} \left(z_k - s(x_k) \right)^2 + \lambda \int_{x_0}^{x_{n-1}} \left(\frac{d^2 s(x)}{dx^2} \right)^2 dx \to \min_{s(x)} \tag{1}$$

with λ being the Lagrange parameter. The above minimization problem can be solved by solving the following linear equations:

$$\left[\mathbf{I} + \alpha^4 \mathbf{Q} \right] \mathbf{s} = \mathbf{z} \tag{2}$$

Where, $\mathbf{I}$ is the identity matrix, $\alpha = 1 \Big/ \left(2 \sin \frac{\pi \Delta x}{\lambda_c} \right)$, λ_c is the cutoff wavelength, $\mathbf{Q}$ is the coefficient matrix depending on the boundary conditions.

The robust spline filter is introduced by minimizing the L1-norm of the residual errors under the condition of minimizing the bending energy and the condition of natural boundary condition. It is defined as:

$$\sum_{k=0}^{n-1} \left| z_k - s(x_k) \right| + \lambda \int_{x_0}^{x_{n-1}} \left(\frac{d^2 s(x)}{dx^2} \right)^2 dx \to \min_{s(x)} \tag{3}$$

This type of minimization problem can be solved by solving the following equation [6]:

$$\left[\beta \alpha^2 \mathbf{P} + (1-\beta) \alpha^4 \mathbf{Q} \right] \mathbf{s} = SGN(\mathbf{z} - \mathbf{s}) \tag{4}$$

The above equation can only be solved iteratively. It is very difficult to find the relationship between the linear and nonlinear spline filters directly, and also the algorithm for solving the nonlinear spline filter can not be found in the literature.

To unify the theory and algorithms of linear and nonlinear spline filters, and to optimize the nonlinear filter by using a better estimator, a generalized spline filter is proposed. It can be defined as the following minimization procedure:

$$\sum_{k=0}^{n-1} \rho\left(z_k - s(x_k) \right) + \lambda \int_{x_0}^{x_{n-1}} \left(\frac{d^2 s(x)}{dx^2} \right)^2 dx \to \underset{s(x_k)}{Min} \tag{5}$$

Comparing this expression with expression (1) and (3), it can be found that the only difference between them is that a more general error metric function $\rho(\cdot)$, which is a symmetric, positive-definite function of the residual error with a unique minimum at zero, is used in the new model.

3. M-estimation

Let r_k be the difference between the k^{th} measurement data z_k and its fitted value s_k. The standard least-squares method tries to minimize $\sum_k r_k^2$, which is not robust if there are outliers present in the data because the objective functions increase indefinitely. The M-estimators try to reduce the effect of outliers by replacing the squared residuals r_i^2 by another function of the residuals, yielding

$$\min \sum_k \rho(r_k) \tag{6}$$

where ρ is a symmetric, positive-definite function with a unique minimum at zero, and is chosen so its rate of increase is less than square when the residual increases. Instead of solving this problem directly, one can implement it as an iterative reweighted least-squares problem. Let $\mathbf{s} = \left[s_0,...,s_{n-1}\right]^T$ be the vector to be estimated. The M-estimator of $\mathbf{s}$ based on the function $\rho(r_k)$ is the vector $\mathbf{s}$ which is the solution of the following n equations:

$$\sum_k \psi(r_k)\frac{\partial r_k}{\partial s_j} = 0, \quad for\ j = 0,...,n-1 \tag{7}$$

where the derivative $\psi(x) = d\rho(x)/dx$ is called the influence function. If we now define a weight function:

$$\delta(r) = \psi(r)/r \tag{8}$$

the equation (7) becomes

$$\sum_k \delta(r_k) r_k \frac{\partial r_k}{\partial s_j} = 0, \quad for\ j = 0,...,n-1 \tag{9}$$

this is exactly the system of equations that we obtain if we solve the following Iterative Re-weighted Least-Squares (IRLS) problem

$$\min \sum_k \delta(r_k^{(m-1)}) r_k^2 \tag{10}$$

here the superscript m indicates the iteration number. The weight $\delta\left(r_k^{(m-1)}\right)$ should be recomputed after each iteration in order to be used in the next iteration.

4. Iteratively Re-weighted Least Square solution for generalised spline filter

According the above discussion of M-estimation theory the minimization problem defined in (5) can be generally solved by using the IRLS method as follows:

$$\sum_{k=0}^{n-1} \delta_k \left(z_k - s(x_k)\right)^2 + \lambda \int_{x_0}^{x_{n-1}} \left(\frac{d^2 s(x)}{dx^2}\right)^2 dx \to \underset{s(x)}{Min} \tag{11}$$

By using Euler-Lagrange calculus,

$$\left[\boldsymbol{\delta}^{(m-1)} + \beta\alpha^2\mathbf{P} + (1-\beta)\alpha^4\mathbf{Q}\right]\mathbf{s}^{(m)} = \boldsymbol{\delta}^{(m-1)}\mathbf{z} \tag{12}$$

Where: $\boldsymbol{\delta}^{(m-1)} = \begin{bmatrix} \delta_0^{(m-1)} & & & & 0 \\ & \delta_1^{(m-1)} & & & \\ & & \ddots & & \\ & & & \delta_{n-2}^{(m-1)} & \\ 0 & & & & \delta_{n-1}^{(m-1)} \end{bmatrix}$ $\mathbf{P} = \begin{bmatrix} 1 & -1 & & & & & 0 \\ -1 & 2 & -1 & & & & \\ & -1 & 2 & -1 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & -1 & 2 & -1 & \\ & & & & -1 & 2 & -1 \\ 0 & & & & & -1 & 1 \end{bmatrix}$ $\mathbf{Q} = \begin{bmatrix} 1 & -2 & 1 & & & & 0 \\ -2 & 5 & -4 & 1 & & & \\ 1 & -4 & 6 & -4 & 1 & & \\ & & \ddots & \ddots & \ddots & & \\ & & 1 & -4 & 6 & -4 & 1 \\ & & & 1 & -4 & 5 & -2 \\ 0 & & & & 1 & -2 & 1 \end{bmatrix}$

Equation (12) can be written more concisely and conveniently as:

$$\left[\mathbf{I} + \beta\alpha^2\mathbf{P} + (1-\beta)\alpha^4\mathbf{Q}\right]\mathbf{s}^{(m)} = \mathbf{s}^{(m-1)} + \boldsymbol{\delta}^{(m-1)}\left(\mathbf{z} - \mathbf{s}^{(m-1)}\right) \tag{13}$$

The other advantage of the equation (13) is that, at every iteration the matrix $\left[\mathbf{I} + \beta\alpha^2\mathbf{P} + (1-\beta)\alpha^4\mathbf{Q}\right]$ is constant and only needs to be calculated once.

4.1. L2 norm - Linear spline filter

Let $\rho(r) = \frac{1}{2}r^2$, then according to equations (7) and (8), $\delta(r) = 1$, and equation (13) can be simplified as:

$$\left[\mathbf{I} + \beta\alpha^2\mathbf{P} + (1-\beta)\alpha^4\mathbf{Q}\right]\mathbf{s}^{(m)} = \mathbf{z} \tag{14}$$

Thus, the superscript m can be removed. Solving equation (14) only one step is needed, it is equivalent to the linear spline filter as defined in the ISO standard.

4.2. L1 norm - Nonlinear spline filter

Let $\rho(r)$ be the L1-norm: $\rho(r) = |r|$, according to equation (7) and (8): $\delta(r) = 1/|r|$, one has:

$$\left[\mathbf{I} + \beta\alpha^2\mathbf{P} + (1-\beta)\alpha^4\mathbf{Q}\right]\mathbf{s}^{(m)} = \mathbf{s}^{(m-1)} + \frac{\left(\mathbf{z} - \mathbf{s}^{(m-1)}\right)}{\left|\mathbf{z} - \mathbf{s}^{(m-1)}\right|} \tag{15}$$

Let SGN be the sign function and ignore the superscript, equation (15) can be simplified as: $\left[\beta\alpha^2\mathbf{P} + (1-\beta)\alpha^4\mathbf{Q}\right]\mathbf{s} = SGN(\mathbf{z} - \mathbf{s})$, which is same as the robust spline filter as drafted in the ISO standard.

4.3. Proposed nonlinear spline filter

Other widely used M-estimators including Huber, Cauchy, and Tukey functions. Among them the Tukey function has been verified to be highly robust against outliers and converges very well [2].

$$\rho(r) = \begin{cases} \frac{c^2}{6}\left(1 - \left[1 - (r/c)^2\right]\sqrt{3}\right), if\ |r| \le c \\ c^2/6, if\ |r| > c \end{cases} \quad \psi(r) = \begin{cases} r\left[1 - \left(\frac{r}{c}\right)^2\right]^2, if\ |r| \le c \\ 0, if\ |r| > c \end{cases} \quad \delta(r) = \begin{cases} \left[1 - \left(\frac{r}{c}\right)^2\right]^2, if\ |r| \le c \\ 0, if\ |r| > c \end{cases} \tag{16}$$

In this paper Tukey function have been chosen as the standard error metric.

5. Experimental results and discussion

The developed linear and nonlinear robust spline filters are applied to some measured data. The processed results are shown in figure 1 and figure 2. Figure 1 shows that the linear spline filter can process data with significant form component very well, and with no boundary effect. Figure 2 is used to compare the linear and nonlinear spline filter. The left and the right figures are the results from a measured honing surface profile and a measured worn milled surface profile respectively. The upper figures show the original profile and the mean profile by using linear and nonlinear spline filters respectively; and the lower figures show the residual profiles. From these figures one can clearly see that both the linear and nonlinear spline filters can follow large form well with almost no boundary effects, while the nonlinear spline filters are robust against data outliers(extremely high peak or deep valley). Also the computation speed is very fast. For a typical 64,129 pts dataset, the linear spline filter only takes 16ms, while the nonlinear spline only needs two iterations to get the converge result (32ms).

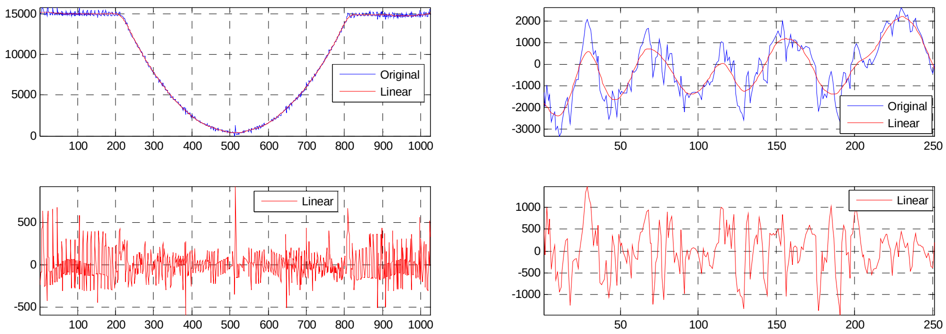

Fig.1 linear spline filter (left: mirolens mould profile, right: chattered milled profile)

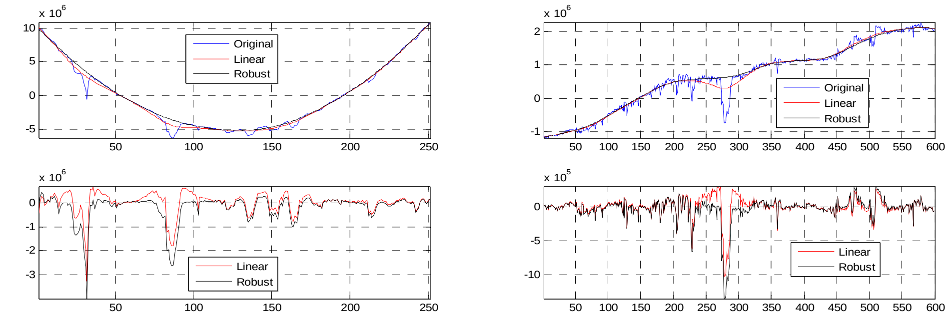

Fig.2 linear and nonlinear spline filter (left: honing surface profile, right: worn milled surface profile)

6. Conclusions

A new generalised spline filter is proposed based on M-estimation theory. Both the linear and nonlinear spline filters can be deduced directly from the general model. The algorithms for the new model based on the IRLS are also very general, effective, efficient and very fast.

Acknowledgements

The authors would like to thank the EPSRC in the UK for support funds to carry out this research work under its programme EP/F032242/1, and the ERC under its programme 228117. The author Xiangqian Jiang would also like to gratefully acknowledge the Royal society for a Wolfson-Royal Society Research Merit Award.

References

[1] X. Jiang, P. Scott, D. Whitehouse, L. Blunt, Paradigm shifts in surface metrology Part I: historical philosophy, Proc. R. Soc., 463(2007) 2049-2070
[2] S. Brinkmann, H. Bodschwinna, Accessing roughness in three-dimensions using Gaussian regression filter, Int. J. of Mach. Tools & Manuf., 41(2001) 2153-2161
[3] J. Seewig, Linear and robust gaussian regression filters, Journal of Physics: conference series, 13 (2005) 254-257
[4] W. Zeng, X. Jiang, P. J. Scott, S. Xiao, L. Blunt, A Fast Algorithm for the High Order Linear and Nonlinear Gaussian Regression filter, Proc. of EUSPEN2009 (accepted).
[5] M. Krystek, Form filtering by splines, Measurement, 18(1996) 9-15.
[6] ISO/DTS 16610-32:2002 Geometrical Product speciation – Filtration, Part 32 : Robust profile filters: Spline filters.
[7] T. Goto, J. Miyakura, K. Umeda, S. Kadowaki, K. Yanagi, A robust spline filter on the basis of L2-norm, Precision engineering, 29 (2005) 157-161.