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REGULARISED DIFFERENTIATION OF MEASUREMENT DATA

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Abstract – The paper is devoted to the numerical differentiation of measurement data. A new method, based on analytical differentiation of the least-squares approximation of data by means of shifted trigonometric functions, is proposed. It is compared with the most popular method of central difference and with a specialised version of the Kalman filter. Some conclusions, concerning metrological applicability of all three methods, are drawn.

Keywords: measurand reconstruction, numerical differentiation, regularisation

1. INTRODUCTION

The topic of numerical differentiation of error-corrupted data is "hot" since the average number of significant publications devoted to it grew from *ca.* 1.5 per year in the decade 1991–2000 to *ca.* 7 per year in the decade 2001–2010 [1]. This may be at least partially explained by a rapid growth of measurement applications where numerical methods of dynamic measurand reconstruction [2] are used – the methods which by principle must contain explicit or implicit differentiation of measurement data.

The recent paper [3] contains an overview and comparison of several classes of regularised methods for numerical differentiation of error-corrupted data, *viz.*:

- the analytical differentiation of the least-squares polynomial or spline approximation,
- the solution of an inverse problem using the Tikhonov or total variation regularisation,
- the method of convolution smoothing with a Friedrichs mollifier,
- the Knowles and Wallace variational method.

In this paper, three alternative methods are assessed, *viz.*:

- the most popular method of central difference (including the optimisation of the differentiation step),
- a new method based on analytical differentiation of the least-squares approximation of data by means of shifted trigonometric functions;
- a specialised version of the Kalman filter.

The reported study has been motivated by the need to differentiate error-corrupted data, representative of the displacement trajectory of a moving person, to obtain its velocity trajectory, required by the decision-making algorithms in the systems for monitoring elderly and disabled people [4-7].

2. ASSUMPTIONS

Let's assume that the first derivative of the function:

$$y = f(x) \tag{1}$$

continuous with its third derivative, is to be estimated on the basis of the error-corrupted values of $f(x)$, *viz.*:

$$\tilde{y}_n \equiv f(x_n) + \eta_n \quad \text{for} \quad n = 0, ..., N \tag{2}$$

where $x_n = x_0 + n\Delta x$ with $\Delta x \equiv (x_N - x_0)/N$, and η_n are realisations of identical, independent, zero-mean random variables $\underline{\eta}_n$ whose standard deviation is σ_η.

3. STUDIED METHODS OF DIFFERENTIATION

3.1. Central-difference method

The central-difference method of numerical differentiation, to be used here as a kind of reference method, is defined by the formula:

$$\hat{y}_n^{(1)} \equiv \frac{\tilde{y}_{n+1} - \tilde{y}_{n-1}}{2\Delta x} \quad \text{for} \quad n = 1, ... N-1 \tag{3}$$

The error of estimation, performed by means of this method, depends on Δx in a way resulting from the proportion of its two parts: a component due to the approximation of the derivative (which is growing with Δx), and a component caused by propagation of the errors corrupting the data to the result of estimation (which is diminishing with Δx). Both those components may be estimated via randomisation of the differentiation formula:

$$\underline{\hat{y}}_n^{(1)} \equiv \frac{\left[y(x_{n+1}) + \underline{\eta}_{n+1}\right] - \left[y(x_{n-1}) + \underline{\eta}_{n-1}\right]}{2\Delta x} \quad \text{for} \quad n = 1, ..., N-1 \tag{4}$$

It can be shown that, if $\sigma_\eta > 0$, the approximation error takes on the form:

$$\Delta\underline{\hat{y}}_n^{(1)} \equiv \underline{\hat{y}}_n^{(1)} - f^{(1)}(x_n) \cong \frac{1}{6} f^{(3)}(x_n)\Delta x^2 + \frac{\underline{\eta}_{n+1} - \underline{\eta}_{n-1}}{2\Delta x} \tag{5}$$

The mean of this error is:

$$\mathrm{E}\left[\Delta\underline{\hat{y}}_n^{(1)}\right] \cong \frac{1}{6} f^{(3)}(x_n)\Delta x^2 \tag{6}$$

and the variance:

$$\mathrm{Var}\left[\Delta\hat{y}_n^{(1)}\right] \cong \mathrm{E}\left[\left(\frac{\eta_{n+1}-\eta_{n-1}}{2\Delta x}\right)^2\right] = \frac{1}{4\Delta x^2} 2\sigma_\eta^2 = \frac{\sigma_\eta^2}{2\Delta x^2} \quad (7)$$

Thus, the dependence of the expanded uncertainty of the derivative estimation on Δx must have a minimum; this means that the differentiation step Δx plays the role of the regularisation parameter in this method of numerical differentiation.

3.2. Proposed method of differentiation

The method presented in this subsection consists in smoothing approximation of the data, followed by analytical differentiation of the result of approximation. It involves the use of approximating functions of the form:

$$\hat{f}(x) \equiv \sum_{k=1}^{K} p_k \varphi_k(x) \quad (8)$$

where:

$$\varphi_k(x) \equiv \varphi(x - x'_k) \quad \text{for} \quad k = 1, ..., K \quad (9)$$

with $\varphi(x)$ being a differentiable compact-support function, and:

$$x_0 \cong x'_1 < ... < x'_K \cong x_N \quad (10)$$

This study is focused on a base function of the form:

$$\varphi(x) \equiv \varphi(x; q, s) = \begin{cases} \cos^{2q}\left(\frac{\pi}{s}x\right) & \text{for } x \in \left[-\frac{s}{2}, +\frac{s}{2}\right] \\ 0 & \text{otherwise} \end{cases} \quad (11)$$

which is continuous with its $q = 1, 2, 3, ...$ derivatives. The first derivative of this function can be calculated using the formula:

$$\varphi^{(1)}(x) \equiv \varphi^{(1)}(x; q, s) =$$

$$= \begin{cases} -2q\frac{\pi}{s}\cos^{2q}\left(\frac{\pi}{s}x\right)\tan\left(\frac{\pi}{s}x\right) & \text{for } x \in \left[-\frac{s}{2}, +\frac{s}{2}\right] \\ 0 & \text{otherwise} \end{cases} \quad (12)$$

This function and its first derivative are depicted in Fig. 1 and Fig. 2. The method of differentiation, in which the function $\varphi(x)$, defined by (11), is used for approximation, will be hereafter referred to using the acronym AB1.

The least-squares (LS) estimate of the vector of parameters $\mathbf{p} \equiv [p_1 \; ... \; p_K]^T$ has the form:

$$\hat{\mathbf{p}} = \mathbf{\Phi}^+ \cdot \tilde{\mathbf{y}} \quad (13)$$

where $\tilde{\mathbf{y}} \equiv [\tilde{y}_0 \; ... \; \tilde{y}_N]^T$, and $\mathbf{\Phi}^+$ is the Moore-Penrose pseudoinverse of the matrix:

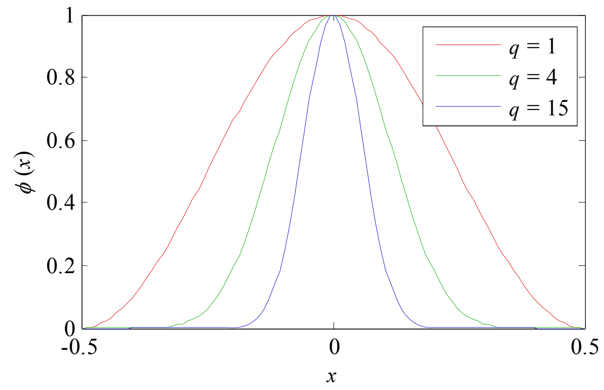

Fig. 1. The function $\varphi(x; q, s)$ for $s = 1$ and three values of q.

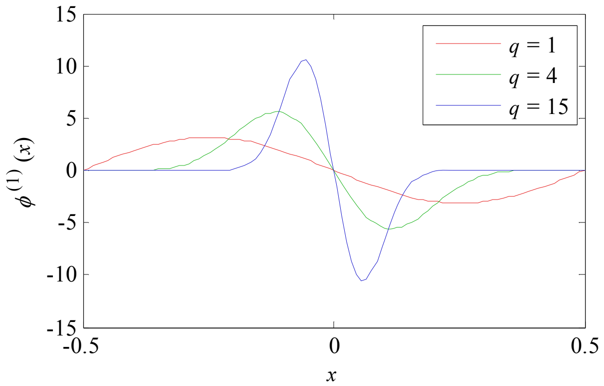

Fig. 2. The first derivative of the function $\varphi(x; q, s)$ for $s = 1$ and three values of q.

$$\mathbf{\Phi} \equiv \begin{bmatrix} \varphi(x_0 - x'_1) & \cdots & \varphi(x_0 - x'_K) \\ \vdots & \ddots & \vdots \\ \varphi(x_N - x'_1) & \cdots & \varphi(x_N - x'_K) \end{bmatrix} \quad (14)$$

The derivative of the function $\hat{f}(x)$ can be calculated in the following way:

$$\frac{d\hat{f}(x)}{dx} = \sum_{k=1}^{K} \hat{p}_k \frac{d\varphi_k(x - x'_k)}{dx} = \sum_{k=1}^{K} \hat{p}_k \varphi^{(1)}(x - x'_k) \quad (15)$$

where $\hat{p}_k$ are elements of the vector of the LS estimates $\hat{\mathbf{p}} \equiv [\hat{p}_1 \; ... \; \hat{p}_K]^T$. Thus, the values of the derivative for $x_0, ..., x_N$ may be computed according to the formula:

$$\hat{\mathbf{y}}^{(1)} = \mathbf{\Phi}^{(1)} \cdot \hat{\mathbf{p}} \quad (16)$$

where:

$$\mathbf{\Phi}^{(1)} \equiv \begin{bmatrix} \varphi^{(1)}(x_0 - x'_1) & \cdots & \varphi^{(1)}(x_0 - x'_K) \\ \vdots & \ddots & \vdots \\ \varphi^{(1)}(x_N - x'_1) & \cdots & \varphi^{(1)}(x_N - x'_K) \end{bmatrix} \quad (17)$$

In the most general case, the parameters K, q and s – as well as the distribution of the points x'_k in the interval $[x_0, x_N]$ – may be used for minimisation of the uncertainty of differentiation. Unfortunately, even for:

$$x'_k = x_0 + (k-1)\Delta x' \quad \text{for} \quad k = 1, \ldots, K \tag{18}$$

with $\Delta x' \equiv (x_N - x_0)/(K-1)$, the analytical joint optimisation of the regularisation parameters (K, q and s) is much more complex than the optimisation of Δx in case of the central-difference method.

Some *a priori* information on the solution may be acquired by means of a simpler method, such as the central-difference method. The result of preliminary differentiation may be useful for diversification of the values of the parameter s after its transformation in a smooth positive envelope (*e.g.* Hilbert envelope); let's denote it with $\breve{y}^{(1)}(x)$. The values $\breve{y}^{(1)}(x'_k)$ may be then used for selection of the parameter s corresponding to $\varphi_k(x)$:

$$s_k = c\,\frac{q\Delta x'}{\breve{y}^{(1)}(x'_k)} \quad \text{for} \quad k = 1, \ldots, K \tag{19}$$

where c is a scalar parameter to be optimised empirically. The matrix $\mathbf{\Phi}$ will, consequently, take on the form:

$$\mathbf{\Phi} \equiv \begin{bmatrix} \varphi(x_0 - x'_1; q, s_1) & \cdots & \varphi(x_0 - x'_K; q, s_K) \\ \vdots & \ddots & \vdots \\ \varphi(x_N - x'_1; q, s_1) & \cdots & \varphi(x_N - x'_K; q, s_K) \end{bmatrix} \tag{20}$$

If available, *a priori* information on the errors in the data may be used for regularisation of the LS method of estimation by replacing the LS formulation of the estimation problem:

$$\hat{\mathbf{p}}_{LS} = \arg_{\mathbf{p}} \min\left\{\left\|\tilde{\mathbf{y}} - \mathbf{\Phi}\cdot\mathbf{p}\right\|_2^2\right\} \tag{21}$$

with the problem of constrained optimisation:

$$\hat{\mathbf{p}}_{CLS} = \arg_{\mathbf{p}} \inf\left\{\left\|\mathbf{\Phi}^{(1)}\cdot\mathbf{p}\right\|_2^2 \;\middle|\; \left\|\tilde{\mathbf{y}} - \mathbf{\Phi}\cdot\mathbf{p}\right\|_2^2 \le \sum_{n=0}^{N} \sigma_n^2\right\} \tag{22}$$

where $\sigma_n^2 \equiv \mathrm{Var}[\eta_n]$. The solution of the latter satisfies the equation:

$$\left(\mathbf{\Phi}^T \cdot \mathbf{\Phi} + \alpha \cdot \mathbf{\Phi}^{(1)T} \cdot \mathbf{\Phi}^{(1)}\right)\cdot \mathbf{p}(\alpha) = \mathbf{\Phi}^T \cdot \tilde{\mathbf{y}} \tag{23}$$

where $\alpha > 0$ is a regularisation parameter. The latter may be selected in various ways, but the discrepancy principle [8] seems to be a good starting point:

$$\hat{\alpha} = \arg_{\alpha}\left\{\left\|\tilde{\mathbf{y}} - \mathbf{\Phi}\cdot\mathbf{p}(\alpha)\right\|_2^2 = \sum_{n=0}^{N} \sigma_n^2\right\} \tag{24}$$

Another estimate of the derivative may be obtained by using linear combination defined by (8), with the function $\varphi(x)$ defined by (11), for approximation of the derivative of $f(x)$ rather than of this function itself. This could be done by using:

$$\varphi_k(x) \equiv \varphi^{(-1)}(x - x'_k) \quad \text{for} \quad k = 1, \ldots, K \tag{25}$$

where $\varphi^{(-1)}(x)$ is the integral of $\frac{2}{s}\varphi(x)$ defined by (11), which can be calculated according to the formula:

$$\varphi^{(-1)}(x) \equiv \varphi^{(-1)}(x; q, s) = \\ = \begin{cases} 0 & \text{for } x < -\frac{s}{2} \\ 2^{-2q}\binom{2q}{q}\left(x + \frac{s}{2}\right) + w(x; q, s) & \text{for } x \in \left[-\frac{s}{2}, +\frac{s}{2}\right] \\ \varphi^{(-1)}\left(\frac{s}{2}; q, s\right) & \text{for } x > \frac{s}{2} \end{cases} \tag{26}$$

where $w(x; q, s) \equiv 2^{-2q}\frac{s}{\pi}\sum_{l=0}^{q-1}\binom{2q}{l}\frac{1}{q-l}\sin\left[2(q-l)\frac{\pi}{s}x\right]$.

This function is depicted in Fig. 3. The method of differentiation, in which the function $\varphi^{(-1)}(x)$ is used for approximation, will be labelled hereafter with the acronym AB2.

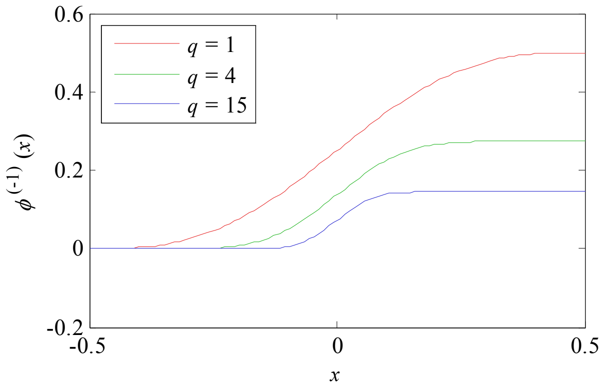

Fig. 3. The function $\varphi^{(-1)}(x; q, s)$ for $s = 1$ and three values of q.

3.3. Kalman-filter-based method of differentiation

The method of numerical differentiation described in this subsection consists in the application of the Kalman filter as defined and studied in [9]. Its specialised version, used in this paper, is based on the following model of the measurement data:

$$\mathbf{y}(n) = \mathbf{F}\cdot\mathbf{y}(n-1) + \mathbf{u}(n-1) \tag{27}$$

$$z(n) = \mathbf{H}\cdot\mathbf{y}(n) + w(n) \tag{28}$$

where $\mathbf{y}(n) \equiv \left[\hat{y}_n \quad \hat{y}_n^{(1)}\right]^T$ with $\hat{y}_n$ and $\hat{y}_n^{(1)}$ being the estimates of y_n and $y_n^{(1)}$, respectively; $z(n) \equiv \tilde{y}_n$, $w(n)$ is the zero-mean random variable with the variance σ_η^2, and $\mathbf{u}(n)$ is a zero-mean random vector with the covariance matrix:

$$\mathbf{Q} \equiv \sigma_u^2 \begin{bmatrix} (\Delta x)^2 & \Delta x \\ \Delta x & 1 \end{bmatrix} \tag{29}$$

where σ_u^2 is a parameter to be optimised empirically. The state-transition matrix $\mathbf{F}$ and the observation matrix $\mathbf{H}$ have the following forms:

$$\mathbf{F} \equiv \begin{bmatrix} 1 & \Delta x \\ 0 & 1 \end{bmatrix} \quad \text{and} \quad \mathbf{H} \equiv \begin{bmatrix} 1 & 0 \end{bmatrix} \tag{30}$$

The result of filtering – an estimate $\hat{y}_n^{(1)}$ of $f^{(1)}(x_n)$ – appears as the second element of the vector $\mathbf{y}(n)$.

4. METHODOLOGY OF COMPARATIVE TESTING

The comparison of the described methods has been based on synthetic data, generated using two functions, defined by the formulae:

$$f_1(t) = t\sin\left(\tfrac{\pi}{2}t\right) \text{ and } f_1^{(1)}(t) = \sin\left(\tfrac{\pi}{2}t\right) + \tfrac{\pi}{2}t\cos\left(\tfrac{\pi}{2}t\right) \tag{31}$$

$$f_2(t) = t^2 \text{ and } f_2^{(1)}(t) = t \tag{32}$$

depicted in Fig. 3 and Fig. 4.

The data – corrupted with additive errors, modelled by pseudorandom numbers – have been generated according to the formula:

$$\tilde{y}_{i,n} = f_i(x_n) + \Delta\tilde{y}_n \quad \text{for} \quad i = 1, 2 \quad \text{and} \quad n = 0, \dots, N \tag{33}$$

where: $\Delta\tilde{y}_n$ are pseudorandom numbers following a zero-mean normal distribution whose standard deviation is σ_η, $x_0 = 0$, $x_N = 5$, $\Delta x = 0.02$ (the number of data in each set: $N+1 = 251$). The sequences $\{\Delta\tilde{y}_n\}$ have been generated in $R = 100$ versions. The derivatives $\hat{y}_{i,n}^{(1)}$ of both functions ($i = 1, 2$) have been estimated on the basis of each version of

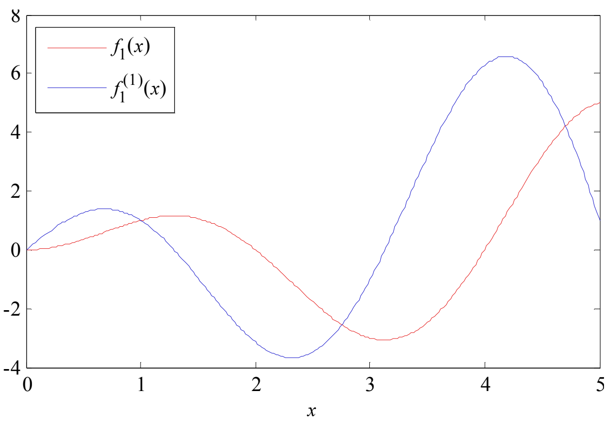

Fig. 3. The function f_1, used for the generation of synthetic data, together with its first derivative.

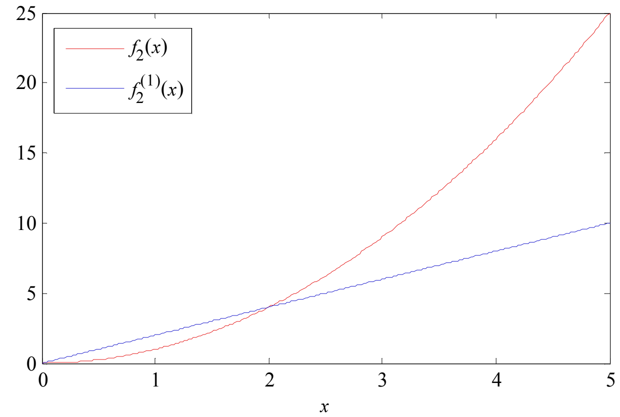

Fig. 4. The function f_2, used for the generation of synthetic data, together with its first derivative.

the data by means of each of the described methods, and the signal-to-noise ratio in the estimates, averaged for the R results, has been used as the criterion of comparison. It has been calculated according to the formula:

$$SNR_1 = 10\log\left(\frac{\sum_{n=1}^{N}\left(\left(f^{(1)}(x_n)\right)^2\right)}{\sum_{n=1}^{N}\left(\left(\hat{f}^{(1)}(x_n) - f^{(1)}(x_n)\right)^2\right)}\right) \tag{34}$$

The experiments have been performed for different values of the standard deviation σ_η characterising the level of noise. For each of those values, the signal-to-noise ratio characterising the data to be differentiated has been calculated according to the formula:

$$SNR_0 = 10\log\left(\frac{\sum_{n=1}^{N}\left(\left(f(x_n)\right)^2\right)}{\sum_{n=1}^{N}\left(\left(\tilde{y}_n - f(x_n)\right)^2\right)}\right) \tag{35}$$

The values of σ_η allowing for obtaining the values of SNR_0 from 5 to 35 dB have been used.

5. NUMERICAL EXPERIMENTS

Figs. 5–8 show the dependence of SNR_1, obtained for the methods AB1 and AB2, on the parameter q, for a fixed value of K, on the basis of data generated using the functions f_1 and f_2, and for two different values of SNR_0. Figs. 9–12 show the results of analogous experiments concerning the dependence of SNR_1 on the parameter K, for a fixed value of q.

In case of the Kalman-filter-based method, the parameter σ_u^2 was optimised empirically, and the value $\hat{\sigma}_u^2 = 0.09$ has been used for experimentation.

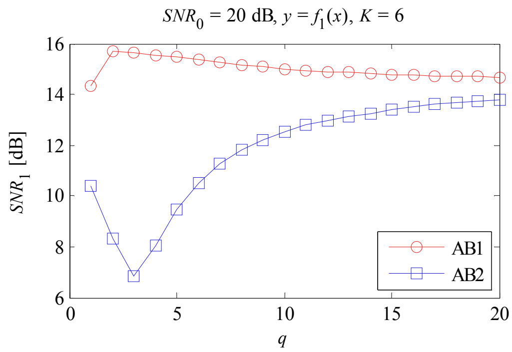

Fig. 5. Dependence of SNR_1 on q for the test function f_1 and for low level of measurement noise.

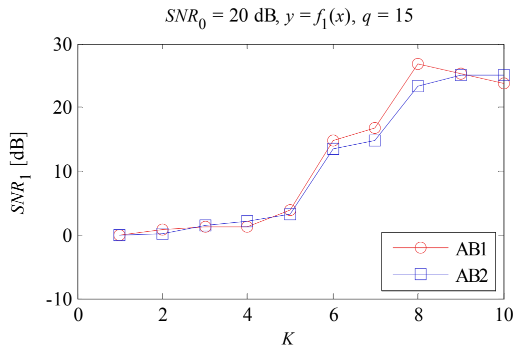

Fig. 9. Dependence of SNR_1 on K for the test function f_1 and for low level of measurement noise.

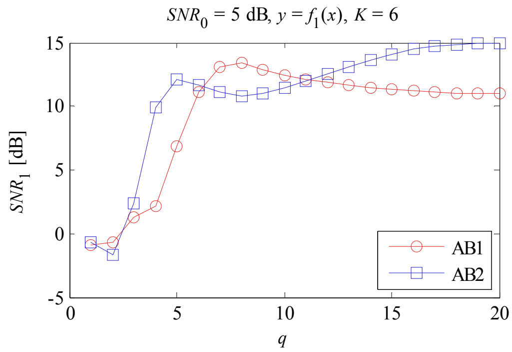

Fig. 6. Dependence of SNR_1 on q for the test function f_1 and for high level of measurement noise.

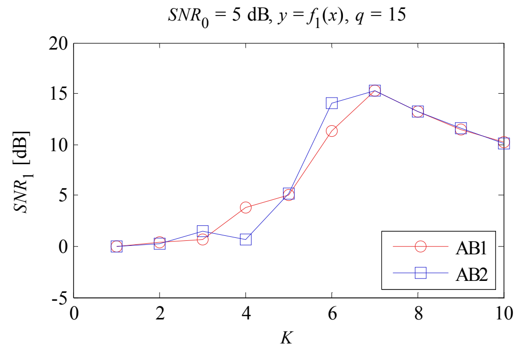

Fig. 10. Dependence of SNR_1 on K for the test function f_1 and for high level of measurement noise.

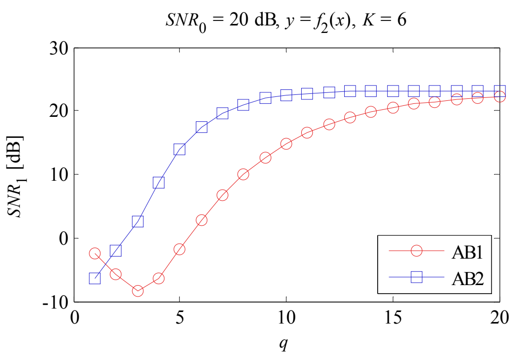

Fig. 7. Dependence of SNR_1 on q for the test function f_2 and for low level of measurement noise.

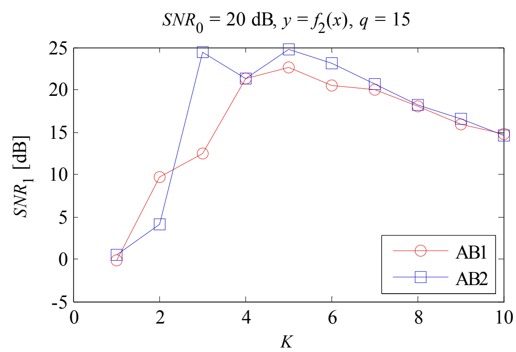

Fig. 11. Dependence of SNR_1 on K for the test function f_2 and for low level of measurement noise.

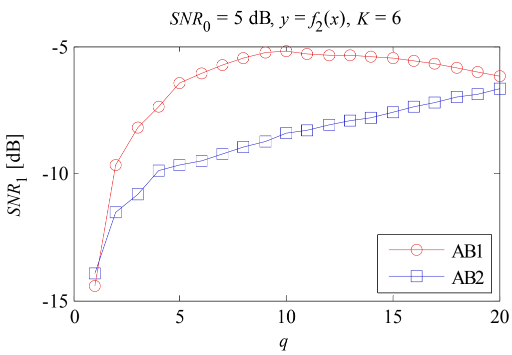

Fig. 8. Dependence of SNR_1 on q for the test function f_2 and for high level of measurement noise.

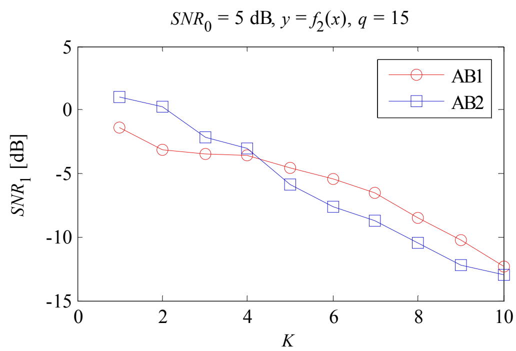

Fig. 12. Dependence of SNR_1 on K for the test function f_2 and for high level of measurement noise.

6. CONCLUSIONS

The results of numerical experiments, presented in the previous Section, indicate that the optimisation of the parameters of the approximation-based methods is a complex issue due to its multidimensionality and to its sensitivity to the properties of the data, such as the level of errors and the shape of the differentiated function. However, on the basis of the presented results, some suboptimal values of the parameters have been selected, *viz.*: $\hat{q} = 15$ and $\hat{K} = 6$. In Fig. 13 and Fig. 14 the dependence of SNR_1 on SNR_0, corresponding to each of the compared methods, is presented.

The results obtained using the test function f_1 demonstrate the superiority of the two approximation-based methods of differentiation for higher-level measurement noise, and of the Kalman-filter-based method of differentiation for lower-level noise. However, in the results obtained using the test function f_2, an opposite trend is demonstrated. All those three methods yield better results than the central-difference method, especially for higher-level measurement noise. Thus, the proposed approximation-based methods might turn out to be useful in some applications; nevertheless, the optimum method of differentiation depends on the sequence of data to be differentiated.

The performance of the method of differentiation, in which the function $\varphi^{(-1)}(x)$ is used for approximation, is quite similar to that of the method in which the function $\varphi(x)$ is used.

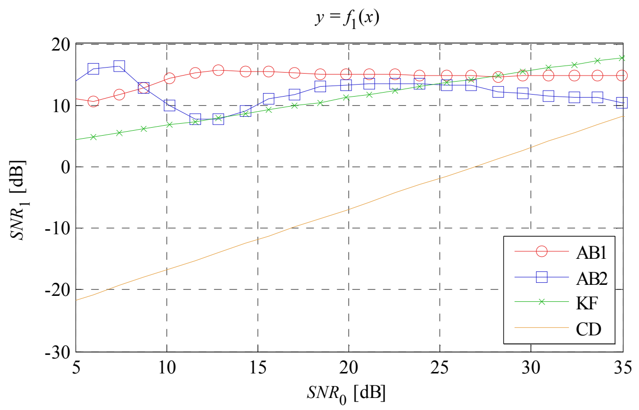

Fig. 13. Dependence of SNR_1 on SNR_0 for the test function f_1: AB1, AB2 – approximation-based methods; CD – central-difference method; KF – Kalman-filter-based method.

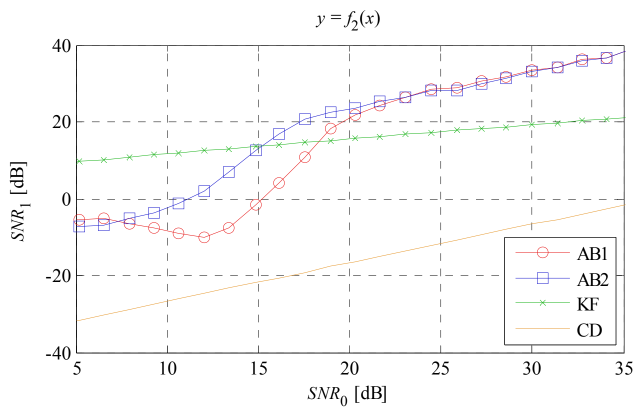

Fig. 14. Dependence of SNR_1 on SNR_0 for the test function f_2: AB1, AB2 – approximation-based methods; CD – central-difference method; KF – Kalman-filter-based method.

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