J. Ind. Geophys. Union ( July 2018 )
**v.22, no.4, pp: 371-378**

# On robust estimation of derivative of noisy dataset: Application on temperature gradient of ocean water column

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**ABSTRACT**
We propose a simple technique of robust estimation of first order derivative of a discrete set of noisy measurements. The proposed technique uses conventional numerical tools, such as the first order finite difference and the natural cubic spline on evenly spaced noisy dataset and provides robust estimation of the first order derivative. We also propose simple techniques in estimating noise level in the measured data. This allows designing the estimated derivative dependent on the noise level in the measured data. We conducted numerical experiments using the proposed technique on synthetic data contaminated with random noise. Results from numerical experiment demonstrate applicability of the technique to the data contaminated with a moderate level of noise. We validate the proposed technique in estimating the temperature gradient of a water column from a set of noisy measurements of temperature versus depth at the northern Gulf of Mexico.

**Key words**: Finite difference, Cubic spline, Robust, Derivative

## INTRODUCTION

Derivative analysis often becomes an essential exercise in various disciplines of earth sciences. The difficulty, one often faces, is lack in robustness in estimating derivative due to the presence of noise in the measured data. To circumvent such difficulty there, in fact, are many numerical methods which claim not only to provide improving precision (Lyness and Molar, 1967; Lele, 1992; Qu, 1996; Shirashi et al., 2007), but also to provide the robustness in the estimating derivative (Anderssen and Bloomfeld, 1974; Cullum, 1971; Wei and Hon, 2005; Chartrand, 2011; Roy, 2015, 2017). Majority of those schemes, as mentioned in the cited literature, have been presented excellently with a full mathematical rigor, but unfortunately such presentations are inconsequential for the researchers, who are not strongly mathematically inclined. On the other hand, a large section of researchers, widely across many scientific fields, are comfortable with the use of a simple difference equation, and the interpolation technique while estimating derivative. The major motivation of the present work is to reduce the communication gap between an excellent theoretician and an avid practitioner in understanding the issue of computational instability in derivative estimation and to provide the necessary remedial measure.

We demonstrate, in this paper, that an appropriate use of a difference equation and selection of an appropriate interpolation technique could be the only two simple elements required in the robust estimation of evenly spaced (mild to moderate level) noisy data. We also demonstrate how the ordeal that an unassuming researcher often faces while estimating the derivative of evenly spaced measured data, using a simple difference scheme. We conducted numerical tests using the proposed scheme on noise contaminated synthetic data in order to demonstrate the applicability of the scheme in estimating derivative of a set of evenly spaced noisy measurements. We next apply the proposed technique in delineating temperature gradient of an ocean water column from northern Gulf of Mexico.

## THEORETICAL BACKGROUND

In an exercise of estimating derivative the premise that we rely on is that the measured data is actually the sample values of a continuous and regular function which is continuously differentiable. Suppose that $f(x)$, defined within an interval $[a,b]$, is one such function such that within a small neighborhood around $x$ the function $f(x)$ can be, decomposed via Taylor series, written as

$$f(x+h) = f(x) + h f^{(1)}(x) + \frac{h^2}{2!} f^{(2)}(x) + \frac{h^3}{3!} f^{(3)}(x) + \cdots, \qquad (1)$$

$$f(x-h) = f(x) - h f^{(1)}(x) + \frac{h^2}{2!} f^{(2)}(x) - \frac{h^3}{3!} f^{(3)}(x) + \cdots, \qquad (2)$$

where $h$ is a small perturbation in $x$, $f^{(1)}$, $f^{(2)}$ and $f^{(3)}$ are the first, second and the third order derivatives of the function $f(x)$ respectively. Using equations (1) and (2) following three difference schemes can be designed to estimate the first order derivative $f^{(1)}$.

Forward difference (I):

$$f^{(1)} = D_h^F\left[f(x)\right] = \frac{f(x+h) - f(x)}{h} + O(h) \qquad (3)$$

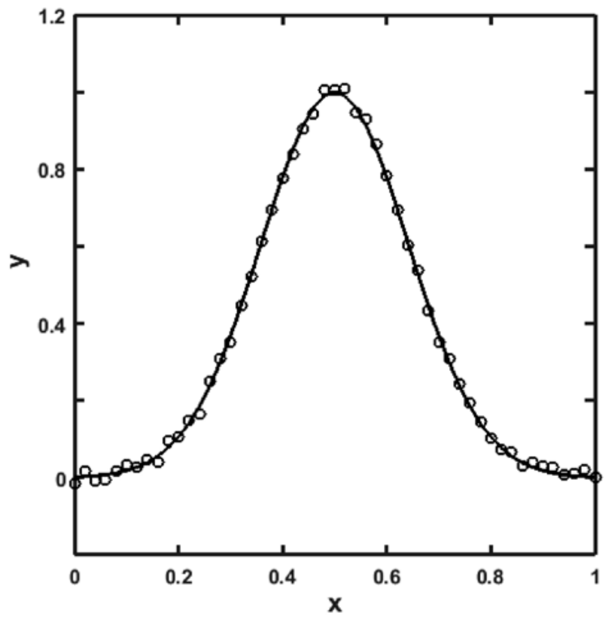


**Figure 1**. Plot of synthetic response (solid line) and the 2% (uniform deviate) random noise contaminated data (open circle). Sampling interval is 0.02.

Backward difference (II):

$$f^{(1)} = D_h^B\left[f(x)\right] = \frac{f(x)-f(x-h)}{h} + O(h) \tag{4}$$

Central difference (III):

$$f^{(1)} = D_h^C\left[f(x)\right] = \frac{f(x+h)-f(x-h)}{2h} + O(h^2), \tag{5}$$

where the symbol 'Big O' in the right hand side of the above three schemes indicates that the error in the precision of estimating derivative is proportional to either $h$ or $h^2$; $D_h^F$, $D_h^B$ and $D_h^C$ denote the forward, backward and central difference operator respectively. If $h$ is small, say a fraction lies between 0 and 1, then the approximation error for the central difference scheme is much smaller compared to the other two schemes, as stated. Note that these are not the only difference schemes in estimating the first order derivatives. There are higher order schemes as well, which offer even much smaller approximation error. One would be tempted enough, in the light of equations (3) to (5), to carrying out measurements as closely as possible; or in other words, maintaining a small data interval, in order to achieve a high level of accuracy in estimating derivative. One would even argue that the smaller the sampling interval in the measurements, larger will be the frequency bandwidth in the measured signal, and hence one should expect a better outcome in estimating derivative of finely sampled data. Such an expectation remains achievable if the set of measurements is completely noise free. Situation, however, changes dramatically the moment a small amount of random noise is incorporated in the measured data. To elucidate it, suppose that the true sampled data $f(x_i)$; $i=1,2,\ldots,n$ contain random noise $e(x_i)$ with the noise amplitude (in terms of r.m.s value) $\delta$ during measurement. Denote the noise contaminated data as $f^\delta(x_i)$ which is equal to $f(x_i) + e(x_i)$, where $e(x_i)$ corresponds to the noise part. The index $i$ denotes the $i$-th instance. Any of the difference operators, as mentioned above, can be used to estimate the derivative. Suppose that the operator $D_h^C$ is used in estimating derivative. Then

$$D_h^C\left[f^\delta(x)\right] = D_h^C\left[f(x)+e(x)\right] = D_h^C\left[f(x)\right] + D_h^C\left[e(x)\right] \tag{6}$$

On what follows, the error in estimating the derivative is now the sum of two components; one is the loss of precision due to the choice of difference operator, which is often termed as consistency error and the other is due to the noise part, commonly called as perturbation error. The noise in data can be realized as wiggles overlain the otherwise smooth data and, supposedly, describe a bounded variation. In the light of equations (3) – (5) the consistency error can be expressed as a non-decreasing function $\varphi(h)$, such that $0 = \varphi(0) < \varphi(h)$ (Lu and Pereverzev, 2006). The perturbation error which arises due to the noise part is, however, proportional to $\delta/h$. Therefore, as the data interval $h$ is becoming small the approximation error due to the loss of precision falls off, but the perturbation error increases in a faster rate. To visualize the effect we give a numerical example, considering a bell-shaped function $\exp[-(x-\mu)^2/2\sigma^2]$, with $\mu=0.5$ and $\sigma=0.02$, defined within an interval [0,1]. The analytical expression of the first order derivative of the bell-shaped (or Gaussian) function is given as $-(x-\mu)^2/2\sigma^2 \exp[-(x-\mu)^2/2\sigma^2]$. The bell-shaped function is digitized with different sampling intervals,

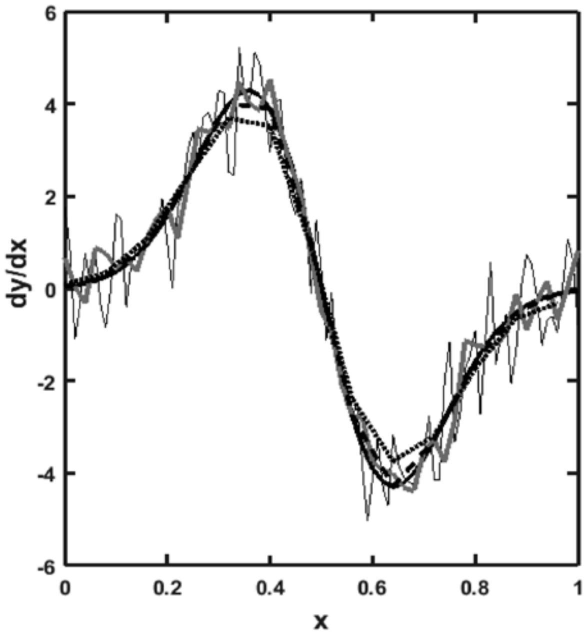


**Figure 2**. Plot of the analytical first order derivative (thick solid line) of synthetic response (Figure 1) and the estimated ones using finite difference schemes for various sampling intervals 0.01 (thin black solid line), 0.02 (thick gray solid line), 0.03 (thick black broken line) and 0.04 (black dotted line).

such as 0.01, 0.02, 0.03 and 0.04, and the digitized data are contaminated with uniformly distributed random noise with a standard deviation ($s$) of 0.02. However, for the sake of clarity only the noise contaminated data (open circle) corresponding to the sampling interval 0.02 and the theoretical response (solid line) and are presented in Figure 1. The figure clearly depicts a realistic situation of measured noisy data. The estimated first order derivative using the difference schemes (I and II for the end points and III for all other points) and the analytical response of derivatives corresponding to three different sampling intervals, as mentioned in the foregoing text, are presented in Figure 2. Consideration of the central difference scheme, except at the end points, for derivative estimation is prompted by the fact that it provides an accurate estimation of derivative than the forward and the backward difference method as truncation error falls of in the power of 2 with respect to the data interval. Note that with the decreasing sample interval, especially at 0.01, the error due to noise component dominates substantially.

However, noise exaggeration is not significant corresponding to the relatively coarse sampling interval (0.04). On the other hand, loss of precision due to coarsening becomes prominent. Results from the numerical experiment with noise contaminated synthetic data corresponding to four distinct sampling intervals clearly suggest that the instability issue in the derivative estimation using a difference scheme can be addressed by increasing the sampling interval or in other words by coarsening the grid while discarding some of the measured data. If such a coarsening can be controlled using the noise level in data (Groetsch, 1991; Ramm and Smirnova, 2001; Lu and Pereverzev, 2006) then a sense of regularization is implied in estimating derivative.

Groetsch (1991) establishes that the regularization in derivative estimation using forward and backward difference schemes is possible if the data spacing $h$ is proportional to $\sqrt{\delta}$. Ramm and Smirnova (2001) suggest that the sampling interval $h$ should be proportional to $\delta^{\gamma}$, where $0<\gamma<1$ in order to ensure regularization in a difference scheme to estimate the first order derivative. Lu and Pereverzev (2006), however, propose a strategy in determining an optimal data spacing in the finite difference based derivative estimation, which is somewhat complicated and computationally involving. According to Lu and Pereverzev (2006) an optimal data spacing, say $h_*$, would be the one which satisfies following condition

*Condition:* Suppose that $\{h_j\}$ for all $j=1,2...$ is a sequence of spacings of a difference grid. A spacing $h_*$ would be an optimal spacing if it is the maximum of all $h_j$ in the sequence so that the discrepancy between the estimated derivative (using any difference scheme) corresponding to $h_j$ and all other estimated derivative previous to the $j$-th one must be less than or (at least) equal to $2a_l\,\delta(1/h_j+1/h_i)$ for $i=1,2,...,j$, where $a_l$ is the absolute sum of the coefficients of an $l$-th order difference equation, such as $a_l = \sum_{j=-l}^{l} |c_j|$. For example, with the first order difference scheme $l=1$, and the coefficients are $c_{-1}, c_0, c_1$.

However, Hanke and Scherzer (2001) argue against regularizing computational regime by means of a coarse discretisation with a view point that discarding data in a grid, in fact, causes loss of information. They also point out that the finite difference approximation essentially renders to the use of piecewise linear or constant functions. They propose to take the route of determining a smoothing function which satisfies the constraint of minimization of an error function, defined in terms of Lagrange's multiplier (or regularization parameter) $\lambda$, and is given as.

$$S[f]=\frac{1}{n-1}\sum_{i=1}^{n}\left(f^{\delta}(x_i)-f(x_i)\right)^2+\lambda\left(\int_0^1\left[f^{(2)}(x)\right]^2dx\right) \tag{7}$$

Once an optimally smoothed function is obtained the robust derivative can be estimated readily. Note that the function which satisfies equation (7) is nothing but a smoothing spline. However, Hanke and Scherzer (2001) demonstrate that as long as the sampling interval $h>\sqrt{\delta/f^{(2)}}$, where $f^{(2)}$ denotes the second order derivative of a smooth and continuously differentiable function, the error bound obtained by a finite difference method and that of the method of the smoothing spline is same. In addition, they also demonstrate that the smoothing functional, thus obtained, satisfying the constraint equation, is actually a natural cubic spline over the grid of sampling points.

## PROPOSED METHOD

In the light of the aforementioned discussion in the earlier section we propose in the following a simple methodology for robust estimation of the first order derivative, given a set of discrete measurements. Instead of providing a garb of mathematical treatment we give a sequential algorithmic pattern (or a work flow).

### Work flow

Get the evenly spaced measured data in a grid $\Delta$ with a known sampling interval $h$.

Get an a priori estimate of the noise level $\delta$ in the measured data.

Piecewise interpolate the measured data using a spline interpolator.

Get the interpolated value at the grid points $x_J$ separated with a grid interval $h_{*}=c\sqrt{\delta}$, where $c\in(0,1]$. The suffix $j$ is used to denote the node corresponding to the new 'coarse' difference grid.

Piecewise interpolate the interpolated values corresponding to the new grid points $x_J$ to the original data grid points.

Compute derivative using a difference schemes (I and II for end points) and III (for all other points).

### Natural spline interpolation

A spline interpolator is actually the major tool of the proposed algorithm in estimating derivative via difference scheme for noisy data. Note that smoothness or regularity is the ultimate attribute of a continuous function to control the wild oscillations what we, generally, observe in estimating derivative of a noisy data. A spline interpolator, which is essentially a piecewise polynomial function demonstrates both the local and the global properties. Locally such a function satisfies every data points while globally, it maintains the regularity condition. A natural cubic spline which possesses the property of continuous second order derivative is widely used spline interpolator and is readily available as a software tool or subroutine function in publicly available open access software, such as PYTHON, OCTAVE, JULIA or as a FORTRAN and C libraries.

### Noise estimation

An a priori knowledge of the noise level in the noise contaminated data is an essential element of the proposed algorithm. Having an a priori knowledge of the noise level in data, in many occasions, especially in earth sciences, is a non-trivial task. This is because, in many occasions, one is forced to have a single set of measurements and hence statistical methods, as available, in the standard text book on statistics, are not applicable in estimating the noise variance in data. For the sake of ease, let us assume that the contaminated noise in data is random and stationary in nature, which means that the noise variance remains fixed for the entire data set. Such assumption, by and large, acceptable in general, although the author agrees that a comprehensive knowledge of noise characteristics requires more elaborate studies. We propose a simple approach in estimating the noise level in a single set of measured data, although such approach does not guarantee providing a precise estimate of the noise level. Presence of random noise causes wiggles in otherwise smooth curve. The smoothest part of a curve is the portion of the curve attaining saturation or becoming flat. In the portion of flat or low slope region the signal-to-noise ratio (SNR) will be very small causing the noise component more prominent. This is the major rationale behind choosing such portion of the curve. The estimated noise variance corresponding to the homogeneous (or nearly homogeneous) regions would lead to estimate the noise level in the data. Following two strategies are proposed:

### Strategy I:

Plot the measured data in X-Y frame and identify the flat or nearly flat portion(s) where the plotted curve would attain saturations. One may use any generic spreadsheet (including open access) software to plot and select a portion of data which corresponds to a nearly flat (or low slope) part of the curve.

If the selected portion of the data is suspected to be reasonably flat then the mean of the selected data would approximately approaches the true value. If the selected data are normalized and the noise, as perceived, is random in nature then the estimated mean would approach the zero value. The estimated variance would then suggest the noise level in data.

If several flat regions in the plotted data are identified then the aforementioned procedure should be continued separately and the average of all estimated noise variance is considered as the best estimated noise variance.

### Strategy II:

If flat or nearly flat region of the plotted data is not identified then choose the portion of the data which seems to be monotonic and corresponds to have mild to moderate slope. Note that the number of data points of the selected region should be at least more than 7 in order to get a reasonable accuracy in the estimation.

Choose a median window of size 3 or 5 and do median filtering by sliding the window every data point and replacing it with the median value. The choice of window size is somewhat ad-hoc, but the guiding principle in selecting an appropriate window size should depend on the noise level in data. The small widow-size works well for data with a low noise level. If the noise level in data is high, a bigger window may be required. For 1D data with the geophysical anomaly the size of the window of a median filter between 3 and 5 is sufficient. The median filter is a sliding window technique where the center of the window should correspond to the data point. The rationale in considering median filter is that it is robust in handling occasional large excursion of data within the selected patch effectively.

We, however, suggest using iterated median filtering on the selected portion of the data set. The pseudo-codes are given below:

Algorithm on iterated median filtering

*Set*: $\mathbf{d}^{\text{old}} = \mathbf{d}^{\delta}$
*Compute*: $\mathbf{d}^{\text{new}} = \text{medianfilter}\ (\mathbf{d}^{\text{old}})$
*Do until*: $\sum_{i=1}^{ns} \left| d_i^{\text{old}} - d_i^{\text{new}} \right| / ns \le \epsilon$, a threshold value $\epsilon \sim 10^{-3}$
*Set*: $\mathbf{d}^{\text{old}} = \mathbf{d}^{\text{new}}$
*Compute*: $\mathbf{d}^{\text{new}} = \text{medianfilter}\ (\mathbf{d}^{\text{old}})$
*End Do*
*Estimate*: $\delta \sim \left\| d^{\delta} - d^{\text{new}} \right\|_{L_2}$.

## NUMERICAL TESTS

### Synthetic data

We conducted numerical experiment to validate the proposed technique of robust estimation of derivative of noisy set of data. For that, we considered synthetically generated data using bell-shaped function. The evenly spaced data ranging within the interval [0,1] are the discrete values of bell-shaped function contaminated with random noise with standard deviation 0.02 are presented in Figure 1. The sampling interval of the digitized data is 0.02. We first attempted to estimate the noise level $d$ in data in order to validate the noise estimation algorithm. The value of the estimated noise level using the Strategy-I for selected data at the left flank of the curve (Figure 3) turns out to be 0.0171, a slight underestimation. The value of the estimated noise level using the Strategy-II on the selected data at the right flank of the curve is 0.0295, a slight overestimation. The average estimated noise level turns out to be 0.0233. The noisy data are piecewise interpolated using natural cubic spline interpolator. We then selected the grid interval $h_*(=c\sqrt{\delta})$ as 0.1202 which corresponds to a set of new spline knots (as presented by large bullets in Figure 3). The knot values are computed using the spline parameters which are already estimated during piecewise interpolation. We then spline fit the estimated data corresponding to the coarse grid interval $h_*$ and get the interpolated data values at the original sampling interval. This gives a smooth estimate of the noisy data. The interpolated curve (solid line) is shown in Figure 3.

To estimate the first order derivative we then used the finite difference schemes, I, II (for the end points) and III (for all other points) corresponding to the original sampling grid. The estimated first order derivative using the proposed algorithm and the synthetic response of the first order derivative are shown in Figure 4.

The estimated mean squared error is given as 0.03267, which suggests a sufficiently robust estimation of the first order derivative of data contaminated with random noise.

### Validation of the method: an example of ocean temperature profile from Gulf of Mexico

The variation of temperature within a column of ocean water plays significant roles in climate research, meteorology and ocean circulation both locally and globally (Helland-Hansen, 1930; Munk, 1966; Stewart, 2008; Williams et al., 2010; Hieronymous et al., 2014). The robust estimate of vertical gradient of temperature depth profile is a key in understanding the movement of water parcel (Stewart, 2008), analyzing the variability of meridional gradient with depth (Roden, 1979), and in making an account of change in temperature due to vertical movement of density surface (Bindoff and McDougall, 1994, Yaremchuk et al., 2001).

We implement the proposed algorithm in estimating the temperature gradient from measured temperature versus depth profile. We chose temperature profile data of a water column at the northern Gulf of Mexico, which is publicly available by US National Ocean and Atmospheric Administration (NOAA). Forrest et al. (2005) compiled and processed 70,000 measurements of mean annual temperature versus depth from 3495 profiles taking an

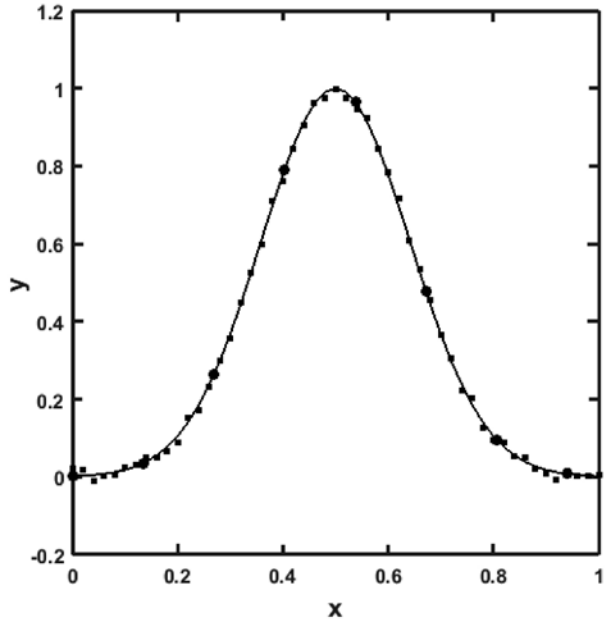


**Figure 3**. Plot of evenly spaced noisy data values (small bullet), interpolated values correspond to coarse grid (large bullet) and final interpolated curve (solid line).

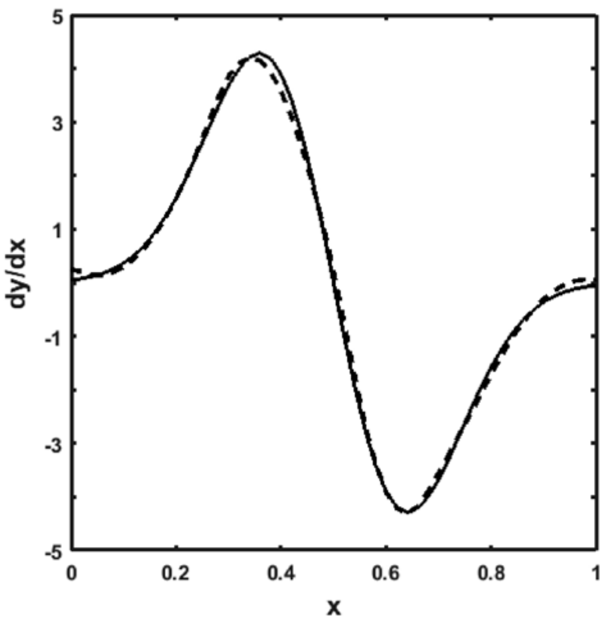


**Figure 4**. Plot of the estimated first order derivative using the proposed algorithm (solid line) and the synthetic response of the first order derivative (broken line).

average from near to ocean surface up to the depth of 5000 feet with a depth interval of 100 ft. We redraw the Figure 3 of Forrest et al., (2005) and digitized it. The original temperature versus depth data are in the units of degree Fahrenheit and foot. We first converted the data into degree Celsius and meter.

The water temperature versus depth profile clearly suggests monotonous decrease in temperature. However, beyond the depth of 1200 meter of the water column such decrease slows down and the curve almost reaches to a flat homogeneous region. We considered a small data sample from the homogeneous region and used the Strategy-I in estimating the noise level in the data. The estimated value of the noise level in data turns out to be 0.0283. We also used Strategy-II in the noise estimation as well. The estimated value of the noise level using Strategy-II is

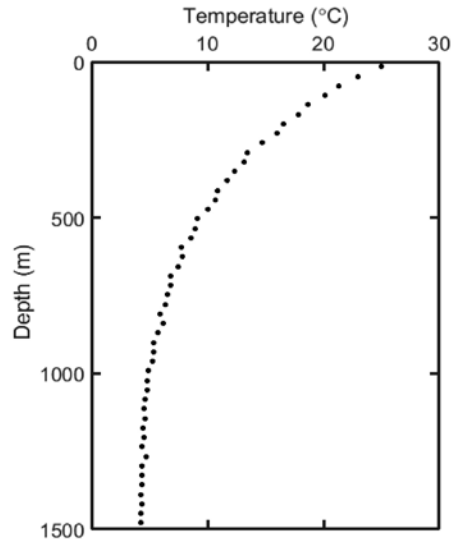


**Figure 5**. Temperature versus depth profile of a water column form the northern Gulf of Mexico, U.S.A.

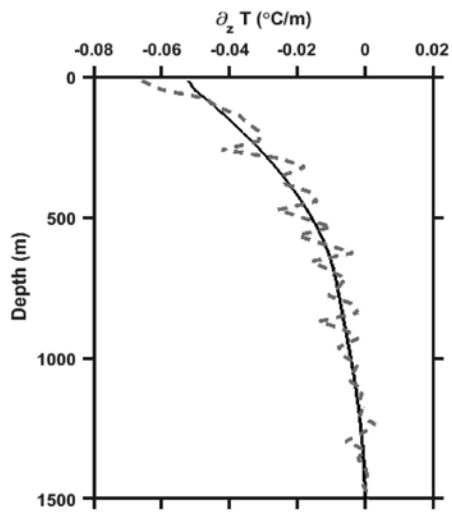


**Figure 6**. Estimated temperature gradient versus depth plot using the proposed (solid line) and the finite difference (gray broken line) scheme on the original data.

0.0274. The average of these two values is 0.02785. The first order derivative which is the temperature gradient $(\partial_z T)$ with depth estimated by the proposed scheme (solid line) and the one estimated using the standard procedure (the finite difference scheme as mentioned in the paper) on the original noisy data (broken line) are presented in Figure 6.

Note that even when the discrete data set contains a moderate level of noise the conventional difference scheme in estimating the first order derivative lacks in robustness. On the other hand, the proposed technique demonstrates sufficient robustness in estimating the first order derivative of a set of evenly spaced noisy measurements. The temperature gradient steadily increases up to a depth of 650 m and attains a plateau there after.

## CONCLUSIONS

The estimation of the first order derivative of a set of measurements is an important exercise to be carried out almost routinely in every field of science including geosciences. A simple technique for robust estimation of derivative of noisy evenly spaced measured data is proposed. The proposed technique which is based on the conventional first order finite difference scheme and cubic spline interpolation technique, demonstrates sufficient robustness in estimating the first order derivative of random noise contaminated synthetic data. A simple strategy (with a workflow) of making an approximate estimate of the noise level in data is discussed. The applicability of the method in estimating the temperature gradient, using temperature versus depth profile data from the northern Gulf of Mexico, is also demonstrated. Most importantly, the proposed technique is so simple that a limited knowledge on numerical methods and an access to the public domain software, such as Python, Octave and Julia is suffice to implement it without much difficulty.

## ACKNOWLEDGEMENT

The author gratefully acknowledges the reviewer, Dr. Simanchal Padhy, for illuminating review which helps significantly in improving the manuscript. The current research is supported by Spaceage Geoconsulting, a research oriented consulting firm.

## Compliance with Ethical Standards

The author declares that he has no conflict of interest and adheres to copyright norms.

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Received on: 18.2.18; Revised on: 30.4.18; Accepted on: 1.5.18