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On the reduced noise sensitivity of a new Fourier transformation algorithm

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On the reduced noise sensitivity of a new Fourier transformation algorithm

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Abstract In this study a new inversion method is presented for performing one dimensional Fourier-transform, which shows highly robust behavior against noises. As the Fourier-transformation is linear the data noise is also transformed to the frequency domain making the operation noise sensitive especially in case of non-Gaussian noise distribution. In the field of inverse problem theory it is well-known that there are numerous procedures for noise rejection, so if the Fourier transformation is formulated as an inverse problem these tools can be used to reduce the noise sensitivity. It was demonstrated in many case studies, that the method of Most Frequent Value provides useful weights to increase the noise rejection capability of geophysical inversion methods. Following the basis of the latter method the Fourier-transform is formulated as an Iteratively Reweighted Least Squares problem using Steiner's weights. Series expansion was applied to the discretization of the continuous functions of the complex spectrum. It is shown that the Jacobian matrix of the inverse problem can be calculated as the inverse Fourier transform of the basis functions used in the series expansion. In order to avoid the calculation of the complex integral a set of basis functions being eigenfunctions of the inverse Fourier transform are produced. This procedure leads to the modified Hermite functions and results in quick and robust inversion-based Fourier-transformation method. The numerical tests of the procedure show that the noise sensitivity can be reduced around an order of magnitude compared to the traditional Discrete Fourier Transform.

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1 Introduction

In geophysical interpretation it is always an important task to reduce the influence of data noises. It is especially true for the continuous Fourier transform as well as its variants the Discrete Fourier Transform (DFT) and the Fast Fourier Transform (FFT) algorithms as they are very sensitive to data noises. To address this problem the Fourier transformation was handled as an over-determined inverse problem (Dobróka et al. 2012), because in the field of geophysical inversion various methods had been developed for noise reduction.

It is well-known from inverse problem theory that simple least square (LSQ) methods give optimal results only when data noises follow Gaussian distribution. The practice of geophysical inversion shows that the least square solutions are very sensitive to sparsely distributed large errors (i.e. outliers in the data set) and the estimated model parameters may even be completely non-physical. More generally, the distribution of the errors in measured data is rarely Gaussian so the use of the LSQ method cannot be optimal which implies the need for a robust inversion method. There are various ways to address the question of the statistical robustness. One of the most frequently used methods in robust optimization is the Least Absolute Deviation (LAD) method. In this case L_1 norm is used to characterize the misfit between the observed and the predicted data. LAD inversion can be numerically realized by using linear programming or (after Scales et al. 1988) applying Iteratively Reweighted Least Squares method (IRLS). Another possibility is the use of the Cauchy criterion (Amundsen 1991). The most popular implementation is the IRLS algorithm involving Cauchy weights. This is a very useful procedure, but it has got a problem that the scale parameter of the Cauchy weights has to be a priori given. This difficulty was elegantly eliminated by Steiner (1988) who derived the scale parameters from the real statistics of the data sets in the framework of the Most Frequent Value method (MFV). It was proved by Dobróka et al. (1991) that the Steiner's weights calculated on the basis of the MFV method results in a very efficient robust inversion method by inserting them into an IRLS procedure. The method was successfully applied in groundwater modeling (by Szucs et al. 2006) and also in constructing and testing a weighted tomography algorithm (W-SIRT) by Dobróka and Szegedi (2014).

To reduce noise sensitivity the Fourier transformation was considered as an overdetermined robust inverse problem using the IRLS method. An essential step of this approach is the use of series expansion in the discretization of the real and imaginary part of the spectrum. Hermite functions were used as basis functions, which gave us the advantage that the elements of the Jacobian matrix can be calculated by means a simple explicit formula. The expansion coefficients were determined in the IRLS algorithm with the use of Steiner's weights.

2 The Fourier transformation and its noise sensitivity

The Fourier transformation plays a very important role in geophysical data processing. By using it the frequency spectrum of the time domain signal can be computed as

$$U(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} u(t) e^{-j\omega t} dt \,, \tag{1}$$

where *u(t)* denotes the time dependent function and *U(ω)* is the complex valued continuous function of frequency (*j* is the imaginary unit). By means of the inverse Fourier transform one can return from the frequency domain to the time domain using the formula

$$u(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} U(\omega) e^{j\omega t} d\omega \,. \tag{2}$$

In the practice of data processing the Discrete Fourier Transform (DFT) and its numerically cost-effective version the Fast Fourier Transform (FFT) is extensively used. In case of a discrete data set the continuous *u(t)* function is sampled in (-T,T) with Δt sampling interval and its DFT is calculated by

$$U(n\Delta f) = \Delta t \sum_{k=\lfloor -N/2 \rfloor}^{\lfloor N/2 \rfloor} u(k\Delta t) e^{-j\frac{2\pi nk}{N}} \,,\ \Delta f = \frac{1}{N\Delta t} \,,$$

where the symbol $\lfloor N/2 \rfloor$ denotes the integer part and *n* is an integer in the $[\lfloor -N/2 \rfloor, \lfloor N/2 \rfloor]$ interval.

2.1 Numerical investigation

In order to demonstrate the noise sensitivity of DFT a numerical experiment is presented. A synthetic data set is calculated equidistantly in the [-1, 1] time interval using the time dependent function

$$u(t) = \kappa t^{\eta} e^{-\lambda t} \sin(\omega t + \phi)\,, \tag{3}$$

where t is the time (in seconds), $\kappa \approx 738.91$ and $\eta = 2$ are constant, $\lambda = 20$ [1/sec], $\omega = 40\pi$ [1/sec], $\varphi = \pi/4$ and the sampling interval is $\Delta t = 0.005$ second. Figure 1 shows this noise-free data set and Fig. 2 represents the real and imaginary part of the spectrum calculated by means of DFT. Two noisy data sets were generated. In case of data set I. the noise-free data shown in Fig. 1 were contaminated by Gaussian noise with zero mean and standard deviation $\sigma = 0.01$. The noisy signal and its DFT are shown in Fig. 3 and Fig. 4, respectively. Data set II. contains noise following Cauchy distribution (with scale parameter $\varepsilon=0.04$, local parameter is zero). The noisy signal and its DFT are shown in Fig. 5 and Fig. 6, respectively.

The distance between the noisy and noise-free data sets is characterized in the time domain by

$$d = \sqrt{\frac{1}{N_t}\sum_{k=1}^{N_t}\left(u^{(noisy)}(t_k) - u^{(noise-free)}(t_k)\right)^2} \qquad (4)$$

and similarly the distance between the (DFT) spectra calculated by means of noise-free and noisy data is characterized by

$$D = \sqrt{\frac{1}{N_f}\sum_{i=1}^{N_f}\left\{\left(\mathrm{Re}\left[U^{(noisy)}(f_i) - U^{(noise-free)}(f_i)\right]\right)^2 + \left(\mathrm{Im}\left[U^{(noisy)}(f_i) - U^{(noise-free)}(f_i)\right]\right)^2\right\}}\ , \qquad (5)$$

where N_t and N_f are the number of the samples in time and frequency domain, respectively. (Throughout the paper the *D* quantity is used as a measure characterizing the noise sensitivity of the method used to calculate the spectrum.) In the present numerical example the $N_t = N_f = 401$ and the characteristic distances are shown in Table 1.

Table 1 Characteristic distances between the noise-free and noisy data in time and frequency domains, respectively.

	data set I. (Gaussian noise)	data set II. (Cauchy noise)
Distance in time domain (d)	0.1032	0.4554
Distance in frequency domain (D)	0.0103	0.0457

3 Methodology

In order to reduce the influence of noise on FT the Fourier transform is treated as an over-determined inverse problem. As a first step the continuous function *U(ω)* should be discretized and written in the form of series expansion

$$U(\omega) = \sum_{n=1}^{M} B_n \Psi_n(\omega) , \qquad (6)$$

where B_n represents the complex expansion coefficients, $\Psi_n(\omega)$ is the n-th known basis function and M is the number of unknown series expansion coefficients. Using the terminology of discrete inverse problem theory, the theoretical (calculated) values of time domain data (forward modeling) can be given by the inverse Fourier transform

$$u^{(calc)}(t_k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\sum_{n=1}^{M} B_n \Psi_n(\omega) \right) e^{j\omega t_k} d\omega = \sum_{n=1}^{M} B_n \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi_n(\omega)\, e^{j\omega t_k} d\omega \quad , \qquad (7)$$

where t_k is the k-th time sample. Let us introduce the Jacobian matrix

$$G_{k,n} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi_n(\omega)\, e^{j\omega t_k} d\omega = \mathcal{F}^{-1}\left\{ \Psi_n(\omega) \right\} , \qquad (8)$$

which is the inverse Fourier transform of the basis function $\Psi_n(\omega)$. Thus, a very simple direct problem is obtained in which theoretical (calculated) data can be written as a linear expression for the B_n expansion coefficients

$$u^{(calc)}(t_k) = \sum_{n=1}^{M} B_n\, G_{k,n}\,, \tag{9}$$

where the unknown model parameters B_n will be estimated by solving an inverse problem.

3.1 A useful choice of basis functions

From Eq. (6) it is obvious that the calculation of the complex integral can be avoided if the basis functions $\Psi_n(\omega)$ are chosen from the eigenfunctions of the inverse FT, that means

$$G_{k,n} = \mathscr{F}^{-1}\left\{\Psi_n(\omega)\right\} = \lambda\, \Psi_n(t_k),$$

where λ is the eigenvalue. It can be proved (Vaidyanathan 2008) that if $\Psi_0(\omega)$ is eigenfunction of $\mathscr{F}^{-1}$ with the eigenvalue λ, then

$$\Psi_1(\omega) = \omega\, \Psi_0(\omega) - \frac{d\Psi_0(\omega)}{d\omega} \tag{10}$$

is also eigenfunction with eigenvalue $j\lambda$, so that

$$\mathscr{F}^{-1}\left\{\Psi_1(\omega)\right\} = j\lambda\Psi_1(t)\,. \tag{11}$$

This expression gives a way to define a set of eigenfunctions. Let us choose

$$\Psi_0(\omega) = e^{-\omega^2/2}\,, \tag{12}$$

which is an eigenfunction of $\mathcal{F}^{-1}$ with $\lambda = 1$

$$\mathcal{F}^{-1}\left\{e^{-\omega^2/2}\right\} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\omega^2/2} \, e^{j\omega t} d\omega = e^{-t^2/2} \ .$$

According to Eq. (7)

$$\Psi_1(\omega) = \omega\Psi_0(\omega) - \frac{d\Psi_0(\omega)}{d\omega} = (2\omega)\, e^{-\omega^2/2}$$

$$\Psi_2(\omega) = \omega\Psi_1(\omega) - \frac{d\Psi_1(\omega)}{d\omega} = (4\omega^2 - 2)\, e^{-\omega^2/2}$$

$$\Psi_3(\omega) = \omega\Psi_2(\omega) - \frac{d\Psi_2(\omega)}{d\omega} = (8\omega^3 - 12\omega)\, e^{-\omega^2/2}$$

etc. are also eigenfunctions of $\mathcal{F}^{-1}$ with eigenvalue j^n in case of $\Psi_n(\omega)$. It can be seen that the sequence of polynomials (in parenthesis) follows the formula

$$h_{n+1}^{(0)}(\omega) = 2\omega\, h_n^{(0)}(\omega) - 2\,n\, h_{n-1}^{(0)}(\omega)\,,$$

which is the recursion equation of the Hermite polynomials with $h_0^{(0)} = 1,\ h_1^{(0)} = 2\omega$. Based on Eq. (12) the desirable set of basis functions in Eq. (6) resulting the form $e^{-\omega^2/2}\, h_n^{(0)}(\omega)$. Using the integral property of the Hermite polynomials

$$\int_{-\infty}^{\infty} e^{-\omega^2}\, h_n^{(0)}(\omega)\, h_m^{(0)}(\omega)\, d\omega = 2^n\, n!\sqrt{\pi}\delta_{nm}\,,\ \delta_{nm} = \begin{cases} 0, n \neq m \\ 1, n = m \end{cases},$$

one can write the basis functions in the orthonormal and square-integrable form of Hermite-functions

$$H_n^{(0)}(\omega) = \frac{e^{-\omega^2/2}\, h_n^{(0)}(\omega)}{\sqrt{\sqrt{\pi}\, n!2^n}}\,,$$

where $h_n^{(0)}(\omega)$ is the n-th Hermite polynomial. It can be seen that the above procedure leads to the well-known result (Duoandikoetxea, 1995) that the Hermite functions are eigenfunctions of the inverse FT

$$\mathcal{F}^{-1}\left\{H_n^{(0)}(\omega)\right\} = (j)^n\, H_n^{(0)}(t)\,. \tag{13}$$

With any other choice of $\Psi_0(\omega)$ (having inverse FT) new sets of eigenfunctions can be defined.

Solving real problems in Fourier transformation the Hermite functions have to be properly scaled, because in geophysical applications the frequency covers a wide range. The scaled Hermite polynomials are introduced by the Rodriguez formula

$$h_n(\omega,\alpha) = (-1)^n e^{\alpha\omega^2}\left(\frac{d}{d\omega}\right)^n e^{-\alpha\omega^2} \tag{14}$$

fulfilling the recursion equation

$$h_{n+1}(\omega,\alpha) = 2\omega\alpha\, h_n(\omega,\alpha) - 2\,n\alpha\, h_{n-1}(\omega,\alpha)$$

and

$$\int_{-\infty}^{\infty} e^{-\alpha\omega^2}\ h_n(\omega,\alpha)\, h_m(\omega,\alpha)\, d\omega = \sqrt{\frac{\pi}{\alpha}}(2\alpha)^n\, n!\,\delta_{nm}\,,\ \delta_{nm} = \begin{cases} 0, & n \neq m \\ 1, & n = m \end{cases},$$

where α is the scaling factor and $h_0(\omega,\alpha)=1,\ h_1(\omega,\alpha)=2\alpha\omega$ (Gröbner and Hoffreiter 1958). So the scaled Hermite functions can be defined as

$$H_n(\omega,\alpha) = \frac{e^{-\alpha\omega^2/2}\, h_n(\omega,\alpha)}{\sqrt{\sqrt{\pi/\alpha}\ n!(2\alpha)^n}}\,, \qquad (15)$$

having the orthogonality equation

$$\int_{-\infty}^{\infty} H_n(\omega,\alpha)\, H_m(\omega,\alpha)\, d\omega = \delta_{nm}\,.$$

The Jacobian matrix based on Eq. (6) can be rewritten by the scaled Hermite functions $H_n(\omega,\alpha)$ *as*

$$G_{k,n} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} H_n(\omega,\alpha)\ e^{j\omega t_k}\ d\omega\,. \qquad (16)$$

Considering the notation $\omega t = \omega' t'$ with $\omega' = \sqrt{\alpha}\omega$, $t' = t/\sqrt{\alpha}$ one can obtain

$$G_{k,n} = \frac{1}{\sqrt[4]{\alpha}} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} H_n^{(0)}(\omega') e^{j\omega' t'_k} \, d\omega' = \frac{1}{\sqrt[4]{\alpha}} \, \mathcal{F}^{-1}\left\{ H_n^{(0)}(t'_k) \right\}, \quad (17)$$

or due to Eq. (13) the complex valued elements of Jacobian matrix can be written directly as

$$G_{k,n} = \frac{j^n}{\sqrt[4]{\alpha}} H_n^{(0)}\left(\frac{t_k}{\sqrt{\alpha}} \right). \quad (18)$$

Thus, the Jacobian matrix can be calculated without integration, which makes the inversion-based Fourier-transform method much quicker. By using Hermite functions as base functions the frequency spectrum is discretized as

$$U(\omega) = \sum_{n=1}^{M} B_n \, H_n(\omega, \alpha) = \sqrt[4]{\alpha} \sum_{n=1}^{M} B_n \, H_n^{(0)}(\omega\sqrt{\alpha}). \quad (19)$$

3.2 The Fourier transform as a Least Squares inverse problem

The discretized form of the spectrum can be written according to Eq. (4) by using the scaled Hermite function system, where the expansion coefficients B_n are calculated in the frame of the over-determined inverse problem. This inverse problem can be highly over-determined if the number of measurement data is much more than that of parameters *($N>M$)*. In case of Least Squares method (LSQ) the L_2 norm of the deviation vector is minimized

$$E_2 = \sum_{k=1}^{N} e_k^2 = \sum_{k=1}^{N} (u_k^{(measured)} - u_k^{(calc)})^2 = \sum_{k=1}^{N} (u_k^{(measured)} - \sum_{n=0}^{M} B_n\, G_{k,n})^2 = \min.$$

The well-known normal equation can be derived from the above condition in the following form

$$\underline{\underline{\mathbf{G}}}^{\mathbf{T}} \underline{\underline{\mathbf{G}}}\, \vec{\mathbf{B}} = \underline{\underline{\mathbf{G}}}^{\mathbf{T}} \vec{\mathbf{u}}^{(measured)} . \qquad (20)$$

(Here $\underline{\underline{\mathbf{G}}}$ is the *NXM* dimensional Jacobian matrix, $\underline{\underline{\mathbf{G}}}^{\mathbf{T}}$ is its transpose matrix, $\vec{\mathbf{B}}$ denotes the *M*-dimensional vector of the unknown expansion coefficients and $\vec{\mathbf{u}}^{(measured)}$ is the *N*-dimensional vector of the time domain data.) After this one can estimate the complex series expansion coefficients

$$\vec{\mathbf{B}} = (\underline{\underline{\mathbf{G}}}^{\mathbf{T}} \underline{\underline{\mathbf{G}}})^{-1} \underline{\underline{\mathbf{G}}}^{\mathbf{T}} \vec{\mathbf{u}}^{(measured)} \qquad (21)$$

and by means of it, the real and imaginary part of the Fourier spectrum can be calculated at any frequency by using Eq. (4). Note, in the knowledge of $\vec{\mathbf{B}}$ the calculated data can be given by Eq. (9) and the estimated spectrum can be computed by means of Eq. (19).

3.2.1 Numerical results with LSQ-FT

In order to test the noise sensitivity of the LSQ inversion based Fourier transform algorithm (LSQ-FT) data sets I. and II. were used as introduced above. The accuracy of the inversion in time- and frequency domains was computed by means of the distances

$$d = \sqrt{\frac{1}{N_t}\sum_{k=1}^{N_t}\left(u^{(estimated)}(t_k) - u^{(noise-free)}(t_k)\right)^2} \tag{22}$$

and

$$D = \sqrt{\frac{1}{N_f}\sum_{i=1}^{N_f}\left\{\left(\mathrm{Re}\left[U^{(estimated)}(f_i) - U^{(noise-free)}(f_i)\right]\right)^2 + \left(\mathrm{Im}\left[U^{(estimated)}(f_i) - U^{(noise-free)}(f_i)\right]\right)^2\right\}} \tag{23}$$

,

respectively. Here $u^{(estimated)}$ and $U^{(estimated)}$ are the time function and frequency spectrum given by means of Eq. (9) and Eq. (19), respectively with the use of the estimated expansion coefficients in Eq. (21). $U^{(noise-free)}$ is calculated by using DFT.

Using $M = 120$ and $\alpha = 0.004$ in case of data set I. the real and imaginary parts of the spectra are shown in Fig. 7. Comparing it to Fig. 4 it can be seen that the LSQ-FT result is less noisy. This is confirmed also by the characteristic distance $D_{I.}^{LSQ} = 0.00614$. Applying the LSQ-FT algorithm to calculate the complex spectrum of data set II., the result is shown in Fig. 8, which seems also very noisy. The characteristic distance calculated by means of Eq. (5) is $D_{II.}^{LSQ} = 0.0229$. This result confirms the well-known fact that the LSQ method gives optimal parameter estimation in case of Gaussian distributed data. In case of both data sets, the LSQ-FT gives better result compared to DFT.

The condition number of the matrix of the normal equation (Eq. (20)) is relatively low ($cond(\underline{\underline{\mathbf{G}}}^{\mathbf{T}}\underline{\underline{\mathbf{G}}}) = 2.0129$) indicating a very stable LSQ inversion procedure. The *M* number of expansion coefficients can be selected in a broad range. In this numerical example using noise-free input data the distances given by Eq. (22) and Eq. (23) (estimation errors) with *M=50* are $d_{noise-free}^{LSQ} = 0.016$ and $D_{noise-free}^{LSQ} = 9.68 * 10^{-4}$, respectively which seems acceptable. Using *M=150* these distances are $d_{noise-free}^{LSQ} = 4.20 * 10^{-4}$ and $D_{noise-free}^{LSQ} = 3.54 * 10^{-4}$. Below *M=50* the estimation of the time function becomes poor, while above *M=150* the numerical accuracy of the calculation of the Hermite functions is rapidly decreasing. The choice of the α parameter is connected also to the numerical accuracy of the calculations as its value determines the range in which the Hermite functions are to be calculated. In the present stage of our research α is chosen in an empirical way. Our experiences shows, that in the interval $(50 \leq M \leq 150)$ the inversion results are acceptable with $(4*10^{-4} \leq \alpha \leq 4*10^{-3})$. To determine the optimal value of α requires further research.

3.3 The Fourier transform as a robust IRLS inverse problem

In order to make the Fourier transform more robust an Iteratively Reweighted Least Squares (IRLS) method using Cauchy weights can also be implemented (Dobróka et al. 2012). In this case the unknown expansion coefficients B_n are estimated by minimizing the weighted norm

$$E_w = \sum_{k=1}^{N} w_k e_k^2 \,, \qquad (24)$$

where the diagonal weighting matrix contains Cauchy weights

$$w_k = \frac{S^2}{S^2 + e_k^2}$$

(with the scale parameter *S*) and the *k*-th element of the deviation vector is

$$e_k = u_k^{measured} - u_k^{calc} \,.$$

As it was mentioned before, there is a problem with inversion procedures involving Cauchy weights: the scale parameter *S* should be a priori given. This difficulty can be solved in the framework of the MFV method (Steiner 1988). In this method the scale parameter ε^2 (Steiner's scale factor called dihesion) is determined in an internal iteration loop. In the *(j+1)*-th step of this procedure the ε_{j+1}^2 can be calculated in the knowledge of ε_j^2 as

$$\varepsilon_{j+1}^2 = 3 \frac{\displaystyle\sum_{k=1}^{N} \frac{e_k^2}{\left(\varepsilon_j^2 + e_k^2\right)^2}}{\displaystyle\sum_{k=1}^{N} \left(\frac{1}{\varepsilon_j^2 + e_k^2}\right)^2} \,,$$

where in the *0*-th step the starting value ε_0 is given as

$$\varepsilon_0 \le \frac{\sqrt{3}}{2}\left(e_{\max} - e_{\min}\right)$$

(Steiner 1988, 1997). It can be seen that the above procedure derives the scale parameter from the data set (deviation between measured and calculated data). The stop criterion can be easily defined by experience (for example, a fixed number of iterations). Using the dihesion given in the last step of the internal iterations Steiner's weights are calculated by using the formula

$$w_k = \frac{\varepsilon^2}{\varepsilon^2 + e_k^2} . \tag{25}$$

In case of Steiner's weights the misfit function given in Eq. (24) is non-quadratic (because e_k contains the unknown expansion coefficients), thus the inverse problem is nonlinear which can be solved again by applying the method of the Iteratively Reweighted Least Squares (Scales et al. 1988). In the framework of this algorithm a *0*-th order solution $\vec{B}^{(0)}$ is derived by using the (non-weighted) LSQ method and the weights are calculated as

$$w_k^{(0)} = \frac{\varepsilon^2}{\varepsilon^2 + \left(e_k^{(0)}\right)^2} \tag{26}$$

with

$$e_k^{(0)} = u_k^{measured} - u_k^{(0)} , \tag{27}$$

where

$$u_k^{(0)} = \sum_{n=1}^{M} B_n^{(0)} G_{k,n} \ . \tag{28}$$

In the first iteration the misfit function

$$E_w^{(1)} = \sum_{k=1}^{N} w_k^{(0)} \left(e_k^{(1)} \right)^2 \tag{29}$$

is minimized resulting in the linear set of normal equations

$$\underline{\underline{\mathbf{G}}}^T \underline{\underline{\mathbf{W}}}^{(0)} \underline{\underline{\mathbf{G}}} \vec{B}^{(1)} = \underline{\underline{\mathbf{G}}}^T \underline{\underline{\mathbf{W}}}^{(0)} \vec{u}^{\,measured} \tag{30}$$

of the weighted Least Squares method where the weighting matrix $\underline{\underline{\mathbf{W}}}^{(0)}$ and its diagonal form

$$W_{kk}^{(0)} = w_k^{(0)} . \tag{31}$$

This procedure is repeated giving the typical *j*-th iteration step

$$\underline{\underline{\mathbf{G}}}^T \underline{\underline{\mathbf{W}}}^{(j-1)} \underline{\underline{\mathbf{G}}} \vec{B}^{(j)} = \underline{\underline{\mathbf{G}}}^T \underline{\underline{\mathbf{W}}}^{(j-1)} \vec{u}^{\,measured} \tag{32}$$

with the $\underline{\underline{\mathbf{W}}}^{(j-1)}$ weighting matrix

$$W_{kk}^{(j-1)} = w_k^{(j-1)} . \tag{33}$$

(In these steps the normal equation is linear, because the weights are always calculated in the previous step. Note that each step of these iterations contains an internal loop for the determination of the Steiner's scale parameter.) This iteration is repeated until a proper stop criterion is met. Finally, in the knowledge of the expansion coefficients the Fourier spectrum can be calculated at any frequency by using Eq. (19) and also the theoretical data set (the inverse Fourier transform) can be calculated by means of Eq. (9).

3.3.1 Numerical results with IRLS-FT using Steiner's weights

In order to test the noise sensitivity of the robust inversion based Fourier transform algorithm (IRLS-FT) at first data set II. was used. The result given in twenty IRLS iterations (with $M = 120$ and $\alpha = 0.004$) is presented in Fig. 9 (the Steiner-weights were computed in an internal loop of ten iterations). Comparing it to Fig. 6 it can be seen that the IRLS-FT algorithm using Steiner's weights gives an improved result, which is confirmed also by the characteristic distance $D_{II.}^{IRLS} = 0.00513$. Note, that this value is (around an order of magnitude) smaller compared to DFT ($D_{II.}^{DFT} = 0.0457$). Similar observations can be made in the time domain by calculating the inverse Fourier transformation using the IRLS-FT spectrum ($u^{(calc)}$ given by Eq. (9)). The result is shown in Fig. 10, which - compared to the input data set II. - demonstrates sufficient noise rejection. This is proved also by the time domain distance between $u^{(calc)}$ and the noise-free data set $d_{II.}^{IRLS} = 0.0381$. (This value should be compared to the distance between data set II. and the noise-free data set shown in Table 1).

The above results demonstrates, that (compared to LSQ-FT) the IRLS-FT algorithm gives better estimation in case of data set containing outliers. It is also important to make the comparison in case of Gaussian data set. For this reason IRLS-FT was applied for the calculation of Fourier spectrum of data set I. The robust IRLS-FT gave slightly worse, but highly acceptable result in case of Gaussian data set with the spectrum distance $D_{I.}^{IRLS} = 0.00649$.

4 Application

It was shown in the previous sections that the inversion-based Fourier transformation can serve as a tool for improving the signal to noise ratio and IRLS-FT using Steiner-weights gives robust Fourier transformation. These features can make the proposed methods promising in various fields of data processing and engineering science.

Some geophysical surveys traditionally require a regular grid along which the measurement data should be collected. Often the temporal and financial effort given for the necessary geodetic measurement exceeds that of the geophysical measurement. On the other hand the modern geophysical instruments have GPS positioning system, giving the possibility to be no longer restricted to measure on equidistant points. To take the advantage of the random walk measurement procedure Sauerländer et al. (1999) published an efficient geomagnetic survey system with avoiding separate geodetic measurement by using GPS in combination with a magnetic instrument and developed new algorithms for triangulation and anomaly detection by using the original, non-gridded data points. The use of non-equidistant measurement arrays obviously needs processing methods independent of the regular or non-regular nature of the sampling.

In the above sections our inversion-based Fourier transform methods were tested on equidistant sampling points. On the other hand it is obvious that the methods do not require equidistant measurement system. To demonstrate it, a random time vector was defined as

$$t_k^{(random)} = t_k^{(regular)} + (rand - 0.5)\,\Delta t\,,$$

where $rand$ is a random number of uniform distribution in the *(0,1)* interval and Δt is the sampling interval. Using this time vector a new data set was calculated by means of Eq. (3). Two noisy data sets were again generated. In case of data set I^r. the noise-free data were contaminated by Gaussian noise with zero mean and standard deviation $\sigma = 0.01$. Data set II^r. contains Cauchy noise with scale parameter $\varepsilon = 0.04$.

Repeating the numerical test with the new data sets very close results were found to our previous investigations. This is proved by calculating the distances

$$D = \sqrt{\frac{1}{N_f}\sum_{i=1}^{N_f}\left\{\left(\mathrm{Re}\left[U^{(random)}(f_i) - U^{(regular)}(f_i)\right]\right)^2 + \left(\mathrm{Im}\left[U^{(random)}(f_i) - U^{(regular)}(f_i)\right]\right)^2\right\}}\,, \qquad (34)$$

where $U^{(random)}(f), U^{(regular)}(f)$ denote the spectrum functions given by our inversion-based FT algorithms using time domain data $u(t^{(random)}), u(t^{(regular)})$ calculated at random or equidistant sampling points (in frequency domain the same data points were used). In case of LSQ-FT the distance given by Eq. (34) was $D_{I^r}^{(LSQ)} = 4.50 * 10^{-4}$, while the IRLS-FT resulted $D_{I^r}^{(LSQ)} = 1.76 * 10^{-3}$. (The distances are so small that the differences in figures can not be visually observed.)

Real field measurements (geomagnetic, gravity, etc.) are usually made on the surface so the data set requires two dimensional data processing and two dimensional Fourier transformation. For this reason the development of our inversion-based FT to the two dimensional applications is in process.

5 Summary and conclusions

The aim of the above considerations was to reduce the noise sensitivity of the traditional Fourier transform. Therefore the FT was formulated as an over-determined inverse problem. In order to discretize the continuous function of the complex spectrum, series expansion was used. It was shown, that the Jacobi's matrix of the inverse problem can be written as the inverse FT of the basis functions used in the discretization. This gave the idea of choosing the basis functions from the eigenfunctions of the inverse FT, as the computation time can be reduced appreciably in this way. Following the procedure of generating eigenfunctions of the FT (Vaidyanathan 2008) is found the scaled Hermite functions are treated as set of basis functions. The unknown parameters (series expansion coefficients) are determined by solving an over-determined inverse problem. Two kinds of inversion procedures were introduced for estimation of the unknowns the LSQ-FT and a robust IRLS-FT. These inversion-based Fourier Transformation methods were tested on synthetic noisy data sets. In order to characterize the accuracy of the methods the characteristic distance between spectra calculated by means of noisy data as well as noise-free ones was applied. The results are summarized in Table 2.

Table 2 Characteristic distances between spectra calculated by means of noisy and noise-free data using DFT, LSQ-FT and IRLS-FT.

	DFT	LSQ-FT	IRLS-FT
Data set I. (Gaussian noise)	0.0103	0.00613	0.00649
Data set II. (Cauchy noise)	0.0457	0.0229	0.00513

The results show that compared to the traditional DFT the noise sensitivity can sufficiently be reduced by using inversion methods. As it is expected, the LSQ inversion gives the best results in the case when the data are contaminated by Gaussian noise and results in moderate accuracy in case of data sets containing outliers (modelled by noisy data following Cauchy distribution). It was shown, that the IRLS-FT method using weights calculated by Steiner's MFV method gives very good estimation results for both Gaussian and Cauchy distributed data noises. Compared to DFT it can result in an order of magnitude improvement in accuracy of the spectrum estimation. Both LSQ-FT and IRLS-FT methods can be applied in non-equidistant measurement arrays.

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Table Captions

Table 1 Characteristic distances between the noise-free and noisy data in time- and frequency domains, respectively.

Table 2 Characteristic distances between spectra calculated by means of noisy and noise-free data using DFT, LSQ-FT and IRLS-FT.

Tables

Table 1 Characteristic distances between the noise-free and noisy data in time and frequency domains, respectively.

	data set I. (Gaussian noise)	data set II. (Cauchy noise)
Distance in time domain (d)	0.1032	0.4554
Distance in frequency domain (D)	0.0103	0.0457

Table 2 Characteristic distances between spectra calculated by means of noisy and noise-free data using DFT, LSQ-FT and IRLS-FT.

	DFT	LSQ-FT	IRLS-FT
Data set I. (Gaussian noise)	0.0103	0.00613	0.00649
Data set II. (Cauchy noise)	0.0457	0.0229	0.00513

Figure Captions

Fig. 1 The noiseless time-domain signal.
Fig. 2 The noiseless frequency domain spectrum.
Fig. 3 The noisy signal containing Gaussian noise (data set I).
Fig. 4 The DFT spectrum of data set I.
Fig. 5 The noisy signal containing noise of Cauchy distribution (data set II).
Fig. 6 The DFT spectrum of data set II.
Fig. 7 The LSQ-FT spectrum of data set I.
Fig. 8 The LSQ-FT spectrum of data set II.
Fig. 9 The IRLS-FT spectrum of data set II.
Fig. 10 IRLS–FT result in the time domain (inverse Fourier transform computed by using IRLS-FT estimated spectrum).

Figures

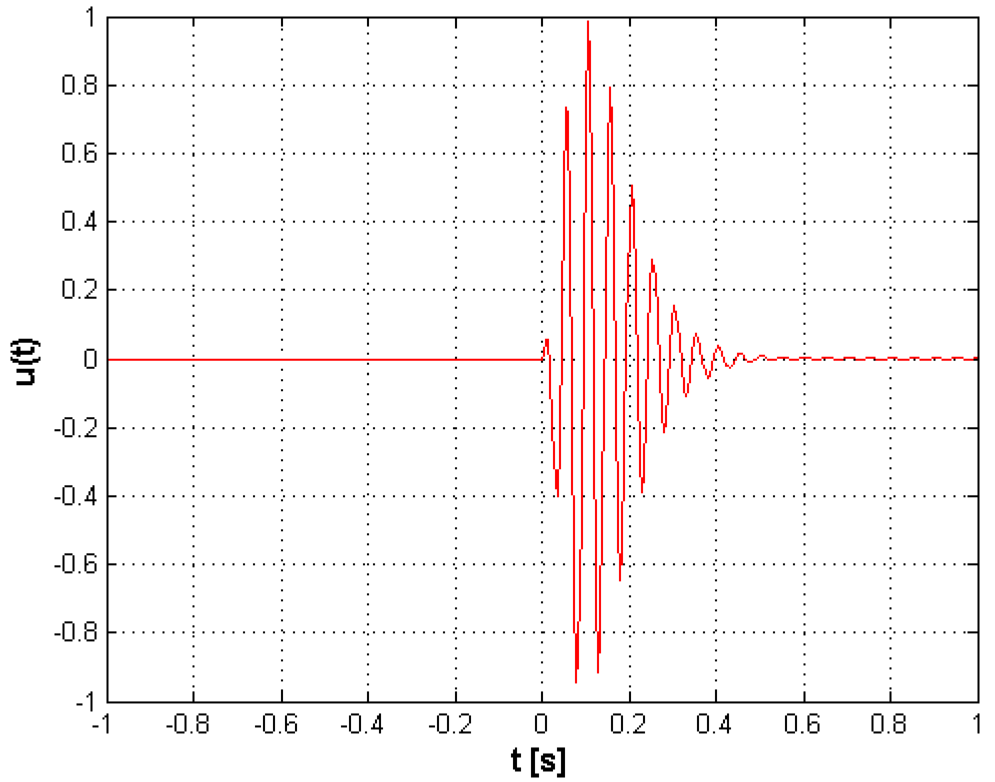

Fig. 1 The noiseless time-domain signal.

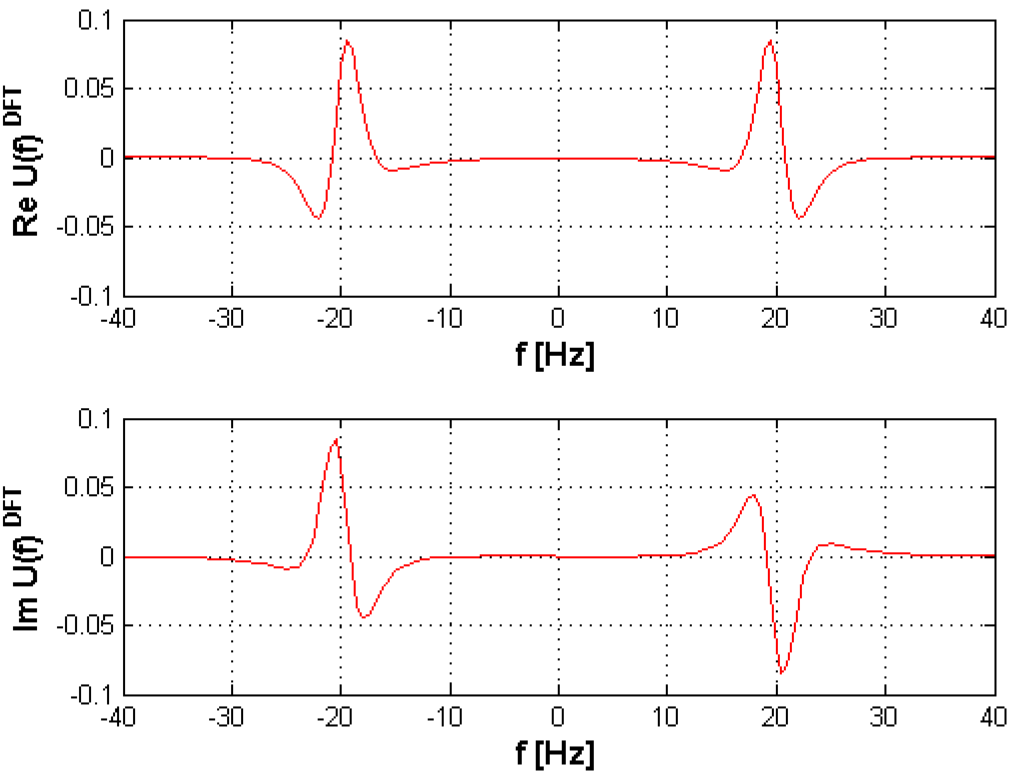

Fig. 2 The noiseless frequency domain spectrum.

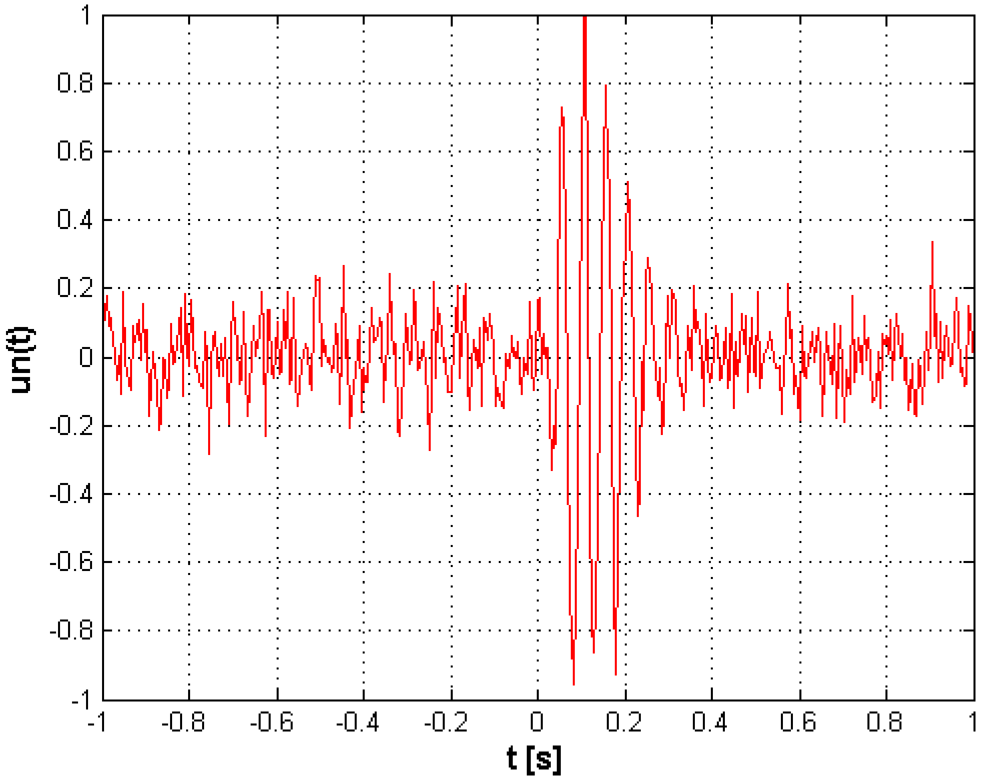

Fig. 3 The noisy signal containing Gaussian noise (data set I).

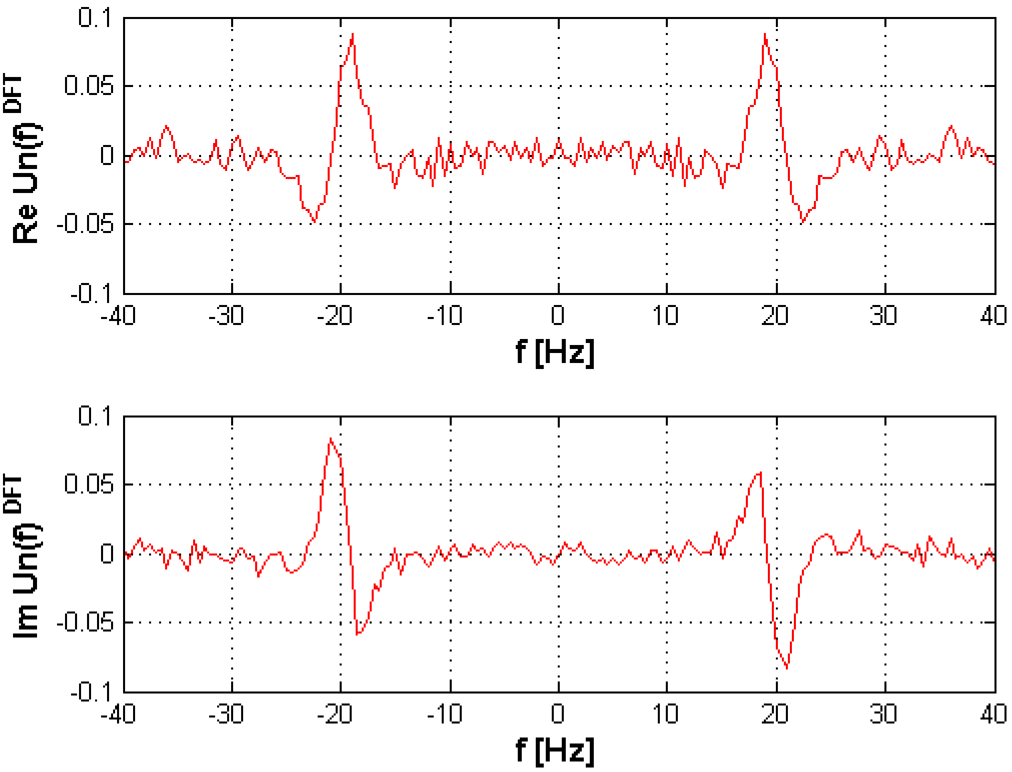

Fig. 4 The DFT spectrum of data set I.

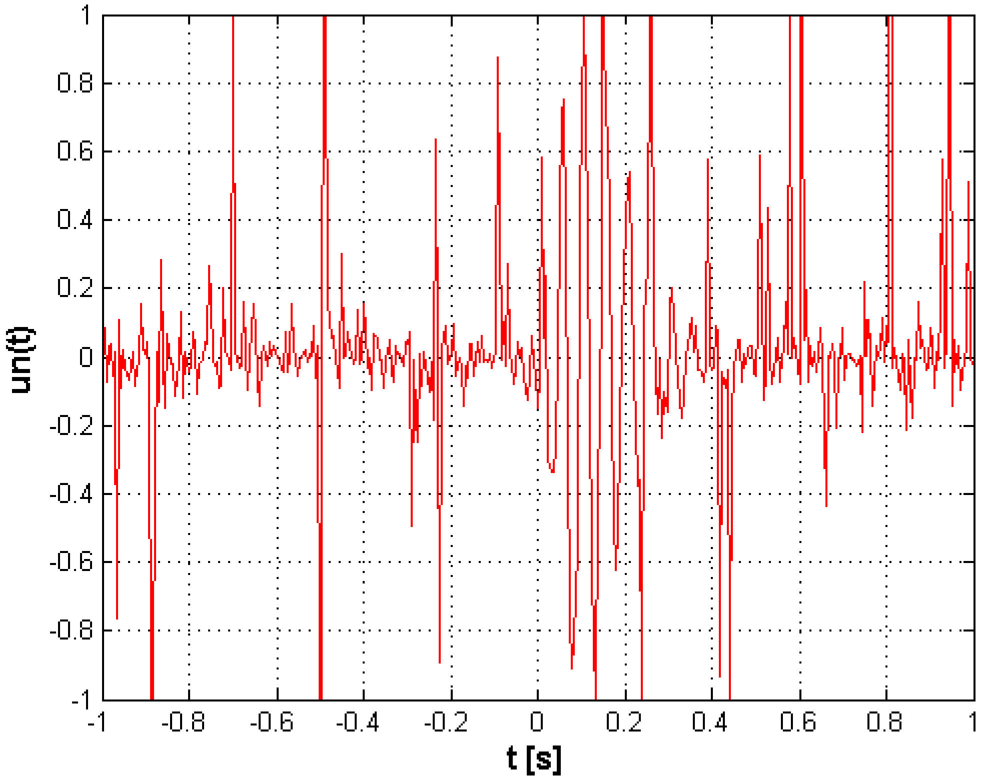

Fig. 5 The noisy signal containing noise of Cauchy distribution (data set II).

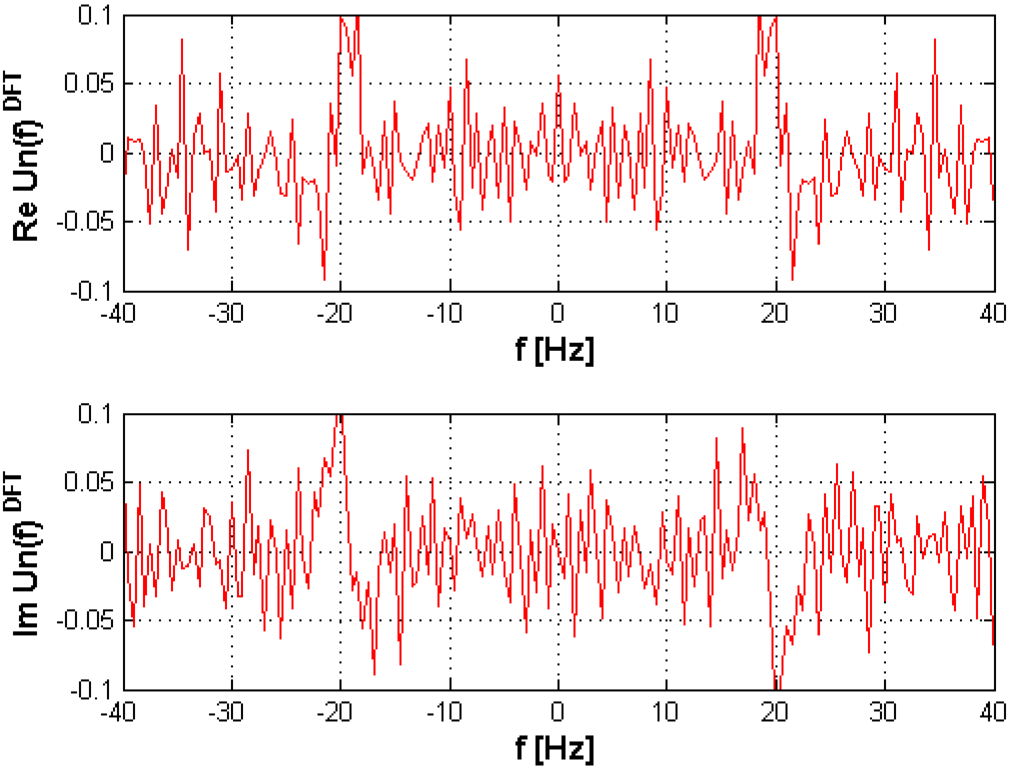

Fig. 6 The DFT spectrum of data set II.

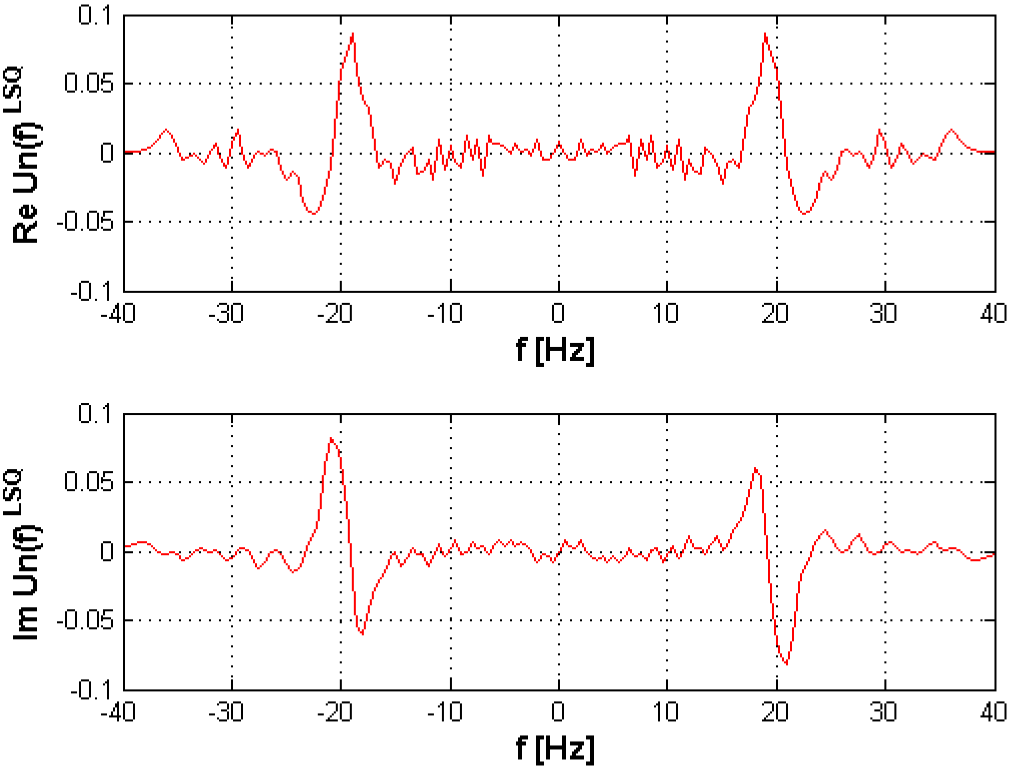

Fig. 7 The LSQ-FT spectrum of data set I.

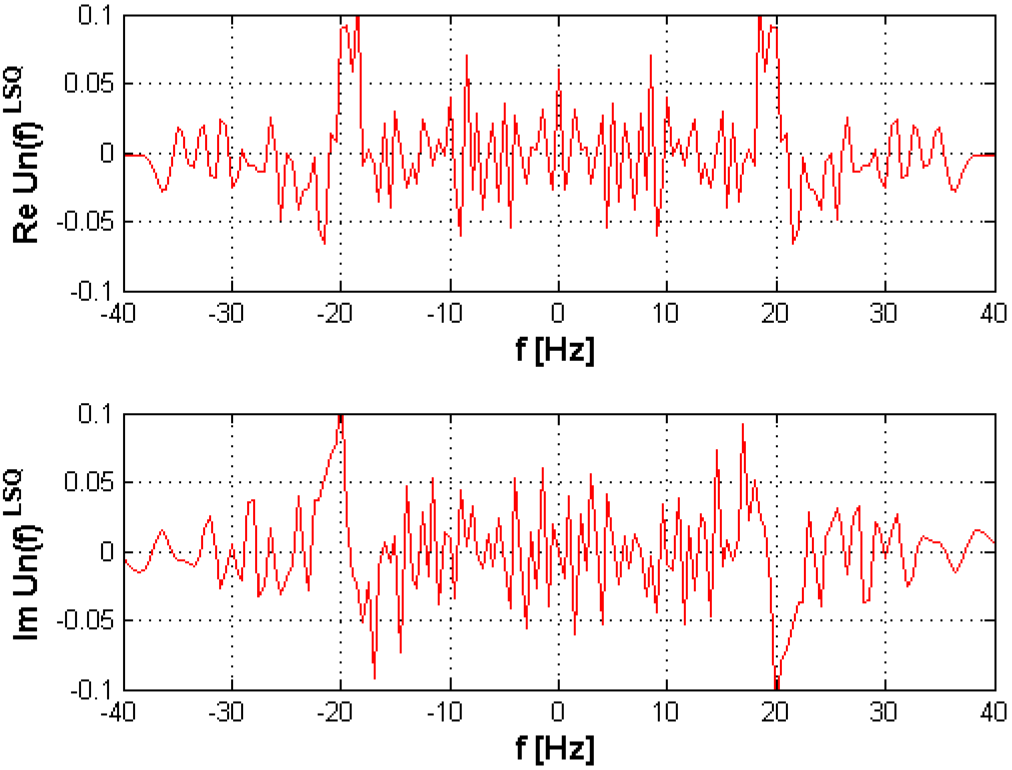

Fig. 8 The LSQ-FT spectrum of data set II.

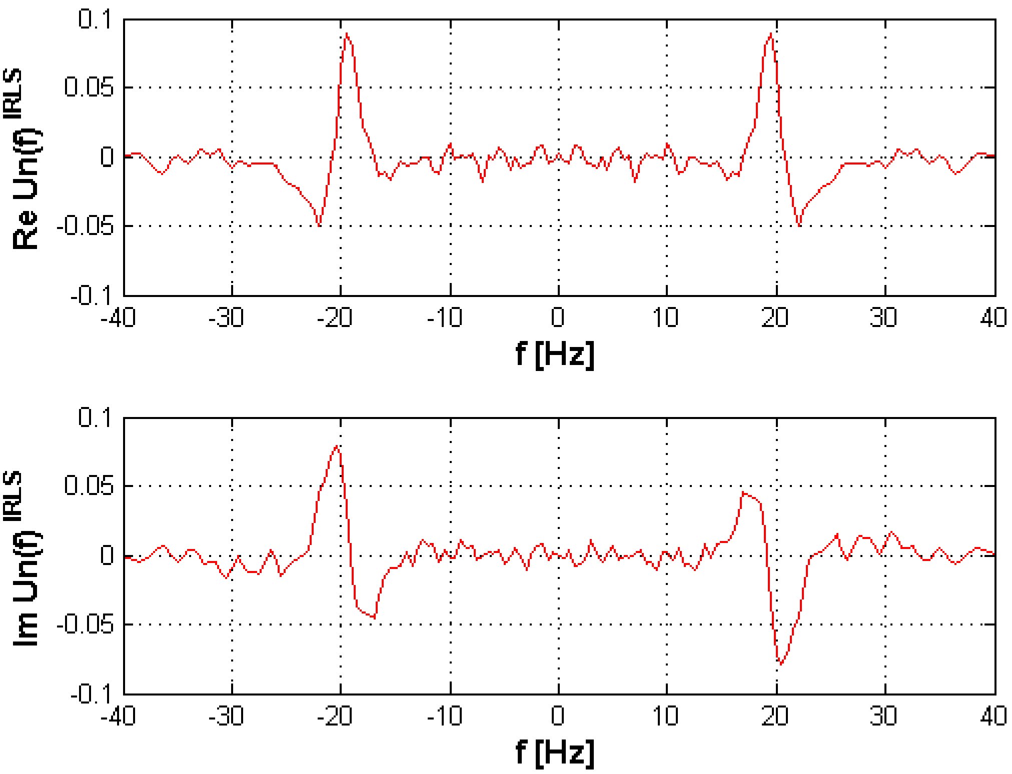

Fig. 9 The IRLS-FT spectrum of data set II.

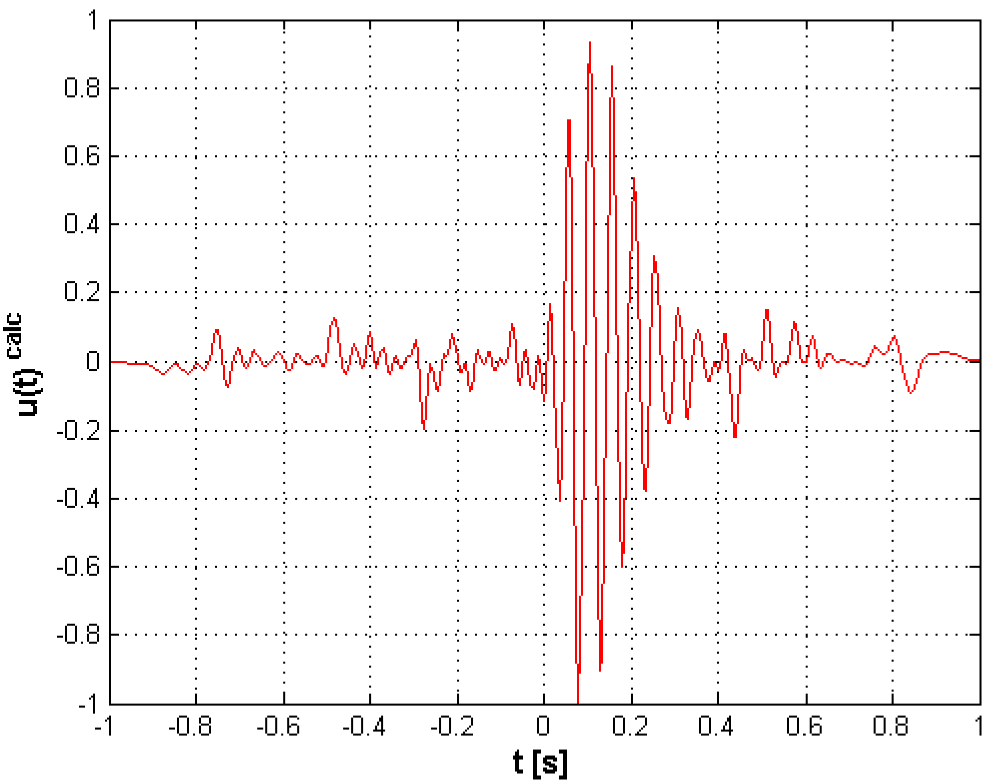

Fig. 10 IRLS–FT result in the time domain (inverse Fourier transform computed by using IRLS-FT estimated spectrum).