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Numerical Problems of Sine Fitting

Algorithms

PhD Thesis booklet

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1 Background and objectives

The thesis deals with numerical problems of sine wave fitting algorithms that are realized with floating-point arithmetic. Sine wave fitting algorithms are applied in several fields of the science of electrical engineering. For instance, the quality of the electrical power system can be characterized with a sinusoidal signal. Furthermore, sine wave fitting opens the door to determine the absolute value and the phase of an impedance. One of the most important application areas is the testing of analog-to-digital converters and of digitizing waveform recorders. The testing methods are prescribed in IEEE standards 1241 and 1057, respectively [1][2].

A general fitted sine wave with arbitrary initial phase and with offset can be described with four parameters, as follows:

$$y_k = A \cdot \cos(2\pi f t_k) + B \cdot \sin(2\pi f t_k) + C, \quad (\text{T.1})$$

where A , B and C denote the amplitudes of the cosinusoidal, sinusoidal and offset (DC) components, respectively, and y_k is the k^{th} sample in the fitted sine wave. The signal frequency is denoted by f . Furthermore, t_k is the time instant at which y_k is evaluated. In the thesis, equidistant (uniform) sampling is assumed. For uniform sampling, time instants are given by

$$t_k = k/f_s, \quad k = 1, \dots, N \quad (\text{T.2})$$

where f_s is the sampling frequency and N denotes the record length. In addition, I also assume that every sample is used in the fitting. In case of equidistant sampling, description can be slightly modified:

$$y_k = A \cdot \cos(\vartheta k) + B \cdot \sin(\vartheta k) + C \quad (\text{T.3})$$
$$\vartheta = 2\pi \frac{f}{f_s} = \frac{\omega}{f_s}$$

where ω denotes the angular frequency, and ϑ is the (to the sampling frequency) relative angular frequency.

The most widely used sine fitting method is the least squares (LS) fitting that minimizes the squared error between the measured and the fitted sine wave. This method is prescribed in [1] and [2]. The cost function (CF) of the LS methods is:

$$\text{CF}_{\text{LS}}(\mathbf{x}, \mathbf{y}) = \sum_{k=1}^N (x_k - y_k)^2 = (\mathbf{x} - \mathbf{y})^T (\mathbf{x} - \mathbf{y}) \quad (\text{T.4})$$

where \mathbf{x} is the measured data and \mathbf{y} is the fitted sine wave.

If parameter ϑ is known, only parameters A , B and C have to be determined. This method is the three-parameter LS fitting (3PLS). If ϑ is unknown, all the four parameters have to be estimated by the four-parameter LS fitting (4PLS). While the 3PLS is linear in the parameters, and can be solved in one step, the 4PLS is non-linear in ϑ . Thus, the estimates of the 4PLS can be obtained with an iterative solution.

Both the 3PLS and the 4PLS methods require the calculation of the Moore-Penrose pseudo-inverse [3]:

$$\boldsymbol{\theta} = \mathbf{D}^+ \mathbf{x} \quad (\text{T.5})$$

where $\boldsymbol{\theta}$ is the parameter vector and \mathbf{D} is the system matrix of the 3PLS or the 4PLS, and operator $^+$ generates the Moore-Penrose pseudo-inverse. Since the 3PLS can be solved in one step, its system matrix is denoted by \mathbf{D}_0 . Contrarily, the 4PLS method is iterative. The system matrix in iteration step i is denoted by \mathbf{D}_i .

The Moore-Penrose pseudo-inverse can be calculated directly by:

$$\mathbf{D}^+ = (\mathbf{D}^T \mathbf{D})^{-1} \mathbf{D}^T . \quad (\text{T.6})$$

However, from a numerical point of view, it may be instable if the condition number of \mathbf{D} is large ($> 10^4$ for single precision, $> 10^8$ for double precision number representation). The condition number is the ratio of the largest singular value to the smallest singular value in the system matrix. This quantity upper bounds the sensitivity of the solution to perturbations. During the fitting, system of equations

$$\mathbf{D}\boldsymbol{\theta} = \mathbf{x} \quad (\text{T.7})$$

has to be solved in LS sense. The condition number of \mathbf{D} gives the upper bound [3]:

$$\frac{\|\boldsymbol{\theta}_\varepsilon - \boldsymbol{\theta}\|_2}{\|\boldsymbol{\theta}\|_2} \leq \text{cond}(\mathbf{D}) \left\{ \frac{\|\mathbf{D}_\varepsilon\|_2 - \|\mathbf{D}\|_2}{\|\mathbf{D}\|_2} + \frac{\|\mathbf{x}_\varepsilon - \mathbf{x}\|_2}{\|\mathbf{x}\|_2} \right\} + O(\varepsilon^2) \quad (\text{T.8})$$

where \mathbf{D}_ε is the perturbed matrix \mathbf{D} , and $\boldsymbol{\theta}_\varepsilon$ is the erroneous solution due to perturbations on \mathbf{D} and \mathbf{x} . In worst case situation, the condition number magnifies these perturbations that may originate, for instance, from roundoff errors. In case of floating point number representation, the magnitude of the perturbation (ε) is the relative error of the number representation (*eps*).

Direct pseudo-inverse calculation may become numerically instable, because the condition number that can be assigned to this method is the square of the condition number of system

matrix \mathbf{D} . In the 4PLS, it can result in the phenomenon that the fitting does not converge. To overcome this problem, decomposition methods, like singular value decomposition (SVD) or QR-decomposition can be utilized [3]. Contrarily, if the condition number of \mathbf{D} is small (<10), direct pseudo-inverse calculation can be applied without numerical issues. This method has the advantage that it is computationally less demanding, compared to decomposition methods.

Increasing the number of samples, the 3PLS (that estimates cosinusoidal, sinusoidal and DC components) remains well-conditioned, while the condition number assigned to the 4PLS (that also estimates signal frequency) increases in portion with the number of samples. Former research in the area showed that with appropriate scaling, under some assumptions, the condition number of the 4PLS can be decreased under 15 [6]. However, accurate upper bounds were not determined neither for the 3PLS, nor for the 4PLS.

In computers, calculations are mostly executed with floating point number representation [4]. In this representation, a number can be given in a form of

$$Sign \cdot M \cdot 2^E \tag{T.9}$$

where M is the mantissa, and E is the exponent. In floating point representation, the representable range is much wider than in fixed point representation. Besides, the relative error of the representation is roughly independent of the absolute value of the number. However, this implies that the larger the absolute value, the larger the absolute error.

The aims of the thesis are the following:

- Find the numerical weak points of least squares sine fitting algorithms that are connected to floating point number representation. Propose methods which can help to decrease these numerical inaccuracies significantly.
- Determine upper bounds on the condition numbers that can be assigned to the 3PLS and the 4PLS methods. Propose methods that ensure that the condition number assigned to the calculation remains small. By this means, numerical inaccuracies in the direct pseudo-inverse calculation can be decreased:

Although the analyses are carried out for the least squares methods, it can be shown that results can be utilized also for the maximum likelihood sine wave estimation [5].

2 Investigation methods

The main goal of the thesis is to find numerical weak points of sine wave fitting algorithms that are implemented with floating point number representation and to give efficient methods in order to ensure that numerical accuracy is improved.

2.1 Phase calculation error

In computers, calculations are mostly executed with floating point representation. This representation has limited relative error, but its absolute error increases with the increasing absolute value of the number to be represented. In order to evaluate sine wave fitting algorithms, the instantaneous phase information has to be determined:

$$\varphi_k = \vartheta k = 2\pi \frac{f}{f_s} k . \quad (\text{T.10})$$

However, this value increases with increasing k . Consequently, at the end of the sampled record, the maximal value of the roundoff error is much larger compared to its value at the beginning, if the number of sampled periods J is large ($J > 10$).

Due to the accumulation of roundoff errors, the results of the CF-minimizer algorithms will be distorted by errors that have much larger amplitudes than the precision of the number representation. Thus, the expected value of the CF is increased, and in the vicinity of the optimum, it behaves as it was disturbed by an additive noise.

In the thesis, I show that due to imprecise phase calculation, roundoff errors that are much larger (even by 4-5 orders of magnitude) than the resolution of the floating point representation, may occur. The roundoff error of the phase calculation is assumed to be white and uniformly distributed in $(-LSB/2; LSB/2]$, where LSB is the value of the least significant bit in the floating point number, that is, the resolution of the represented number. It is derived that in the applicability range of the assumptions, both the expected value and the variance of the CF is increased due to imprecise phase calculation. I show that the increase of the expected value and of the variance is proportional to the number of samples, and proportional to the square of the number of sampled periods J and of the relative error of the number representation (ϵ_{ps}). Thus, increasing J or N , or decreasing floating-point precision increases the expected value and the variance of the CF.

Besides revealing the error source, I also give an efficient method, in order to increase the numerical precision of the evaluation of the instantaneous phase. In the algorithm, the periodic property of sine and cosine functions is exploited. Namely,

$$\sin(\varphi_k) = \sin(2\pi n + \varphi_k) \quad n \in \mathbb{Z} . \quad (\text{T.11})$$

Thus, only the fractional part of the phase information in (T.10) needs to be known in order to calculate sine and cosine values. The proposed method is that the phase information should be calculated by $2\pi \left\langle \frac{f}{f_s} k \right\rangle$, where $\langle \cdot \rangle$ denotes the fractional part after rounding to the nearest integer value. During the calculation, $\frac{f}{f_s} k$ and $\left\langle \frac{f}{f_s} k \right\rangle$ are evaluated with increased precision, and after the evaluation of the fractional part, the result is stored on the original limited precision. Increased precision is needed, because if $\frac{f}{f_s} k$ was evaluated in the standard way, precise phase information would be lost at the storage of the results, due to roundoff errors. With this method, $\left\langle \frac{f}{f_s} k \right\rangle$ is mapped to a limited range $(-0.5; 0.5]$, and the value of the phase information is also be limited to range $(-\pi; \pi]$. Since the roundoff error of floating point representation is roughly proportional to the absolute value of the represented number, with this limitation, the roundoff error is significantly decreased. The advantage of this method is that only the fractional part of the phase is evaluated with increased precision. Thus, the algorithm needs extra computational demand at its numerical weak point. The other parts of the method can be evaluated with the original limited precision.

The naive approach of summation may also result in an error in the fitting. In the naive approach, the next term is added to a growing sum. The effect of this error source on the CF is much smaller than that of the imprecise phase calculation. However, if needed, it can be significantly mitigated by applying pairwise summation [7].

2.2 Upper bound on condition numbers

In the thesis, upper bounds on the condition numbers that can be assigned to the 3PLS and the 4PLS are determined. It is proved that under some assumptions, these condition numbers can be decreased to a small value (< 10). Thus, direct pseudo-inverse calculation can be applied without numerical problems.

I prove that an upper bound on the condition number of the 3PLS can be given that is roughly inversely proportional to the number of sampled periods. To this aim, perturbation theory on eigenvalues is applied [8]. The matrix that determines the condition number of the 3PLS ($\mathbf{D}_0^T \mathbf{D}_0$) can be approximated by a diagonal matrix:

$$\mathbf{H} = \begin{pmatrix} N/2 & 0 & 0 \\ 0 & N/2 & 0 \\ 0 & 0 & N \end{pmatrix}. \quad (\text{T.12})$$

The error of the approximation is represented in matrix \mathbf{E} . Upper bounds on the elements of \mathbf{E} are determined in the thesis. Applying perturbation theory on eigenvalues,

$$|\lambda_i - \tilde{\lambda}_i| \leq \|\mathbf{E}_b\|_F \quad (\text{T.13})$$

where \mathbf{E}_b contains the bounds on the element of \mathbf{E} , $\|\cdot\|_F$ denotes the Frobenius-norm, λ_i is the i th eigenvalue of \mathbf{H} , and $\tilde{\lambda}_i$ is the i th eigenvalue of the $\mathbf{D}_0^T \mathbf{D}_0$. In the thesis, I prove that the same upper bound can be given for the singular values:

$$|s_i - \tilde{s}_i| \leq \|\mathbf{E}_b\|_F \quad (\text{T.14})$$

where s_i is the i th singular value of \mathbf{H} , and \tilde{s}_i is the i th singular value of $\mathbf{D}_0^T \mathbf{D}_0$. Provided that

$$J/N \leq 1/4 \quad (\text{T.15})$$

holds, that is, at least four are sampled from one period, I prove that the condition number assigned to the 3PLS can be upper bounded: it is smaller than 11, if $J > 2$. If J is increased beyond 4, the condition number drops under 3.8. The derived upper bound is roughly inversely proportional to the number of sampled periods.

With a simple modification, the matrix that determines the condition number assigned to the 4PLS ($\mathbf{D}_i^T \mathbf{D}_i$) can also be made approximately diagonal. While running the investigated fitting algorithms, it is usually assumed that the measurement started at time instant $t = 0$. However, the sampled signal is processed offline. Thus, $t = 0$ has no physical meaning, and it can be arbitrarily shifted. With the modification of time axis parameters, $t = 0$ was set so that it is at the middle of the data set. With this data centering, sampling instants of the samples are located symmetrically with respect to this instant. Formally, an offset is subtracted from the ordinal number of the sample (k). The needed time offset (l) can be calculated as:

$$l = (N + 1)/2 \quad (\text{T.16})$$

and the new instantaneous phase is

$$\varphi_{k-l} = \vartheta(k - l) . \quad (\text{T.17})$$

Certainly, this modifies the parameters of the description, but data centering does not influence the fitted sine wave as a time domain signal. This method makes the modified 4PLS matrix ($\mathbf{D}_i^T \mathbf{D}_i$)' approximately diagonal. It can be approximated by

$$\mathbf{H}' = \begin{pmatrix} N/2 & 0 & 0 & 0 \\ 0 & N/2 & 0 & 0 \\ 0 & 0 & N & 0 \\ 0 & 0 & 0 & R^2 S_1 \end{pmatrix} \quad S_1 = \frac{N^3 - N}{24}. \quad (\text{T.18})$$

I prove that if the third column of the modified 4PLS system matrix \mathbf{D}'_i is scaled (divided) by $\sqrt{2}$, and the third column is scaled by $R \sqrt{\frac{N^2-1}{12}}$, then by increasing J , the condition number of the scaled $(\mathbf{D}'_i{}^T \mathbf{D}'_i)'$ matrix reaches its theoretical minimum asymptotically (R is the aggregated amplitude of the investigated sine wave, $R = \sqrt{A^2 + B^2}$).

Data centering can also be applied in case of the 3PLS. In this case, I prove that if the third column of the system matrix is scaled by $\sqrt{2}$, then by increasing J , the theoretical minimum of the condition number assigned to the 3PLS can be reached asymptotically, as well.

3 New scientific statements – Theses

Thesis 1 – I have shown that due to floating point number representation, the evaluation of the instantaneous phase of the sine wave is distorted by roundoff errors that increase with the ordinal number of the sample. These errors increase the expected value and the variance of the least squares cost function. I have calculated the increase in the expected value and in the variance under the following assumptions: the roundoff errors are independent and uniformly distributed, the effects influencing the sine wave are modeled as additive independent noise with uniform or Gaussian distribution.

- 1.1 I have shown that the increase in variance term of the LS cost function that is dominant in practical applications, and the increase in the expected value of the LS cost function can be by more orders of magnitude larger than the roundoff error of the floating point number representation. In the applicability range of the assumptions, these values are approximately proportional to the record length and approximately squarely proportional to the number of sampled periods and to the relative number representation accuracy of the floating point representation.
- 1.2 I have given an effective algorithm in order to increase the accuracy of phase evaluation. This algorithm calculates the instantaneous phase with increased precision. Exploiting the periodicity of sine and cosine functions, the result is mapped to range $(-\pi; \pi]$. The method upper bounds the maximal roundoff error that occurs at the representation of the phase information on finite precision.

Related own publications: [RB1], [RB3], [RB4].

Thesis 2 – I have determined upper bounds on the condition numbers that can be assigned to the three- and four-parameter least squares sine wave fitting algorithms.

- 2.1 I have proved that with equidistant sampling, recording at least four samples from one period, using every sample in the record, the condition number assigned to the standardly formalized three-parameter least squares sine wave fitting method can be upper bounded by

$$\frac{1 + \frac{0.75}{J}}{0.5 - \frac{0.75}{J}}, J > 1.5,$$

where J denotes the number of sampled periods. (Time instants of the standardly given algorithm were determined by formula

$$t_k = \frac{k}{f_s} \quad k = 1 \dots N$$

where f_s denotes the sampling frequency.)

2.2 I have proved that with equidistant sampling, recording at least four samples from one period, using every sample in the record, setting time axis parameters symmetrically with respect to 0, and scaling the DC component of the system matrix by $\sqrt{2}$, the upper bound on the condition number that can be assigned to the three-parameter least squares sine wave fitting algorithm is

$$\frac{0.5 + \frac{0.4}{J}}{0.5 - \frac{0.4}{J}}, \quad J > 0.8.$$

where J denotes the number of sampled periods. By this means, I have proved that by increasing J , the theoretical minimum of the condition number can be reached asymptotically. (By setting time axis parameters symmetrically with respect to 0, sampling instants were calculated by formula

$$t_k = \frac{k - l}{f_s}, \quad k = 1 \dots N, \quad l = \frac{N + 1}{2} .)$$

2.3 I have proved that with equidistant sampling, recording at least four samples from one period, using every sample in the record, setting time axis parameters symmetrically with respect to 0, scaling the DC component of the system matrix by $\sqrt{2}$ and the relative angular frequency component of the system matrix by $R \sqrt{\frac{N^2 - 1}{12}}$, the upper bound on the condition number that can be assigned to the four-parameter least squares sine wave fitting algorithm is

$$\frac{0.5 + \frac{0.98}{J}}{0.5 - \frac{0.98}{J}}, \quad J \geq 4$$

where R is the amplitude of the record, N is the number of samples and, J denotes the number of sampled periods. By this means, I have proved that by increasing J , the theoretical minimum of the condition number can be reached asymptotically. The relative angular frequency is given by

$$\vartheta = \frac{\omega}{f_s}$$

where ω is the angular frequency of the signal. (By setting time axis parameters symmetrically with respect to 0, sampling instants were calculated by formula

$$t_k = \frac{k - l}{f_s} , \quad k = 1 \dots N , \quad l = \frac{N + 1}{2} .)$$

Related own publications: [RB2].

4 Applicability and outlook

In the thesis, I show that imprecise phase calculation and ill-conditioning in the system of equations can significantly decrease the numerical accuracy of the three- and four-parameter least squares sine wave fitting algorithms. I propose solutions that mitigate the effect of both error sources considerably.

By the application of the proposed solutions, it can be certified that the results are not affected by the phase calculation errors. Besides, it can be guaranteed to the user of the algorithm that by fulfilling certain conditions, the assigned condition number remains low. Consequently, the investigated algorithms can be implemented in a numerically robust way even in single precision. Thus, the cost of the equipment that is needed to execute sine fitting, can be reduced significantly.

The results of the thesis can be generalized for linear and non-linear LS fittings. In polynomial fitting – which is the most well-known among linear fitting applications – the method of setting parameters symmetrically with respect to 0 is known in the literature [9]. However, results can also be applied for nonlinear LS fittings, where the nonlinearity is caused by a transcendental function – this happens in case of the 4PLS fitting. An example is the exponential growth:

$$f(z_1, z_2, t) = z_1 \cdot e^{z_2 t} \quad (\text{T.19})$$

where $z_1 > 0$ and $z_2 > 0$ are the parameters of the exponential growth, and t denotes time. Exponential growth can model, for example, the increase in a population. The to be fitted curve is

$$y_k = f(z_1, z_2, t_k) = z_1 \cdot e^{z_2 t_k} . \quad (\text{T.20})$$

If the values of t_k are all positive, the scalar product of the columns that are assigned to z_1 and z_2 in the system matrix can be decreased significantly, by subtracting an offset from t_k . By this means, with proper scaling, the condition number assigned to the algorithm can be decreased, as well.

The decrease of roundoff errors due to imprecise phase calculation can be applied in the area of frequency domain system identification [10], if identification is performed with multisine excitation. With the method proposed in the thesis – ensuring that the roundoff errors due to imprecise phase calculation are reduced before the generation – the errors in the generated multisine can be decreased.

In the thesis, I exploited the periodic property of sine and cosine functions. Thus, only the fractional part of the phase (with respect to 2π) is needed to evaluate the functions. By analogy with this approach, the accuracy of multiplication and raising to power of complex numbers can also be improved. At the multiplication of complex numbers, their absolute values are multiplied, while their phases are added. If the sum of two phases is out of interval $(-\pi; \pi]$, then by increasing the precision of the calculation of the phase information, and mapping the result in the given interval, roundoff errors can be decreased.

The topic of the thesis is related to the research of the researcher group [11], established by Professor István Kollár († 2016). The researcher group is specialized for analog-to-digital converter (ADC) testing. Results of the research are built in the ADC testing MATLAB toolbox. Decrease of the phase calculation error and scaling of the parameters are planned to be included in the toolbox.

The researcher group is in contact with researchers of the Technical University of Košice, University of Perugia and Free University of Brussels (VUB). As a result of the co-operation, several joint publications has been published [RB1],[RB3],[5],[12],[13]. Besides the numerical problems of sine wave fitting, determining the lower bound for the variance of the maximum likelihood sine wave fitting (Cramér-Rao lower bound) and efficient parametrization of this method in order to reduce the parameter space of the estimation are also active research areas. With keeping international contacts, we plan to make further research in this area. In the long run, our aim is to standardize the results of our research in IEEE standard 1241 [1]. This standard contains prescriptions for ADC testing. During further investigations, the underlying ideas of the thesis can be certainly extended to the following areas:

- analysis on condition numbers in case of non-uniform sampling. In this case, the elapsed times between two samples are not equal, for instance, due to jitter;
- investigation of the effect of overdrive or data loss on condition numbers. In this case, there are time instants at which no data are available for the fitting;
- the effect of multi-harmonics on the results;
- determination of scaling factors for the case of the maximum likelihood estimator.

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Related publications

- [RB1] B. Renczes, I. Kollár, A. Moschitta, P. Carbone, “Numerical Optimization Problems of Sine Wave Fitting Algorithms in the Presence of Roundoff Errors”, *IEEE Transactions on Instrumentation and Measurement*, vol. 65, no. 8., pp. 1785-1795, 2016, © IEEE, 2016
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