

Analyzing Numerical Optimization Problems of Finite Resolution Sine Wave Fitting Algorithms

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Abstract—In this paper the numerical behavior of different sine wave fitting methods is investigated. In addition to the Three- and Four-Parameter Least Squares Fits, also the Maximum Likelihood and the Quantile Based Estimator methods suffer from similar numerical problems that may disturb the result of the ADC test. Suggestions are given in order to improve the performance of the investigated algorithms.

Keywords—Analog-Digital Converter Testing, Sine Wave Fitting, Numerical Optimization, Least Squares Fit, Maximum Likelihood Method, Quantile Based Estimator

I. INTRODUCTION

Analog-to-Digital Converters convert the signals of the analog world into digital samples that can be effectively processed with computers. Sine wave fitting algorithms are widely used to be able to verify the quality of the conversion and the converter itself. In the IEEE Standard 1241-2010 the Three- and Four-Parameter Least Squares (LS) Sine Wave Fits are described as test methods. The latter solves a four-parameter problem: fits the signal model

$$x[n] = A \cdot \cos\left(2\pi \frac{f_0}{f_s} n\right) + B \cdot \sin\left(2\pi \frac{f_0}{f_s} n\right) + C \quad (1)$$

to the measured data so that the *Root Mean Square Error (RMS)*, or *Noise and Distortion (NAD)* is minimal:

$$NAD = \sqrt{\frac{1}{N} \sum_{n=1}^N (x[n] - y[n])^2}, \quad (2)$$

where A , B , C , f_0 and f_s are the amplitudes of the fitted cosine and sine components, offset and the frequencies of the signal and of sampling, respectively, N is the number of samples, $x[n]$ is the n^{th} sample of the fitted sine wave, and $y[n]$ is the n^{th} sample in the digitized set of samples. The four-parameter fit optimizes parameters A , B , C and f_0 , while during the three-parameter fit f_0 is assumed to be known exactly [1].

The quality of the analog-to-digital conversion can be characterized by the parameter *ENOB (Effective Number of Bits)*:

$$ENOB = b - \log_2 \frac{NAD}{LSB/\sqrt{12}}, \quad (3)$$

where b is the nominal resolution of the converter in bits [1]. The Least Squares fit yields the highest possible *ENOB*, since it minimizes parameter *NAD*, thus *ENOB* is usually slightly overestimated. Other methods were shown to be able to yield more precise results. The *Maximum Likelihood method* [2] can

estimate three or four parameters, and can even estimate the standard deviation of the additive input noise. The *Quantile-based Estimator* [3] in its current state (restricted to coherent sampling, with repeated samples) fits a three-parameter sine wave to the measured data, based on the Gauss-Markov theorem.

Computers can only execute operations with limited resolution. In PCs IEEE double precision number representation is commonly used, with relative error $eps = 2.22 \cdot 10^{-16}$, while for DSPs single precision is used ($eps = 1.19 \cdot 10^{-7}$). Detailed description of eps can be found [4]. In this article, single precision behavior will be investigated, and double precision will be used for reference values. This is beneficial for two reasons: reference calculations are easily available in double precision, and single precision roundoff is more apparent in experimental investigations. Moreover, in many applications only single precision number representation is available, e.g. for signal processing with DSPs, so it may be desirable to implement algorithms also for this limited precision [5].

The limited resolution results in the following error sources:

- imprecisely stored value of the relative signal frequency (f_0/f_s),
- imprecise evaluation of the phase (the value of the sine depends on the fraction only, i.e. $\sin\phi = \sin\{k2\pi + \text{fract}(\phi, 2\pi)\}$),
- imprecise evaluation of the cost function (CF), or of the gradient, or of the minimizing/maximizing solution. These are closely connected with the summation of many numbers, with the condition number of the equations to be solved, and with the evaluation of the cumulative distribution function (CDF) of the noise.

In Section II the general problem of phase evaluation is investigated which occurs in each investigated algorithm. In Section III numerical problems of each algorithm are highlighted, and suggestions are given for improvement. Finally, Section IV describes how it is possible to increase precision on a given platform.

II. ERROR OF PHASE EVALUATION

Let us consider a sampled sine wave with unit amplitude and zero phase. Let the frequency f_0 be equal to 10 Hz, while the sampling frequency f_s to 1000 Hz:

$$x[n] = 0.5 \cdot \sin(\varphi[n]), \quad (4)$$

$$\varphi[n] = 2\pi \frac{f_1}{f_s} n, \quad (5)$$

where $\varphi[n]$ is the phase of the n^{th} sample and n goes from 1 to N . For this example, let us also consider that we have a lot of samples (1 million). Sampling is coherent, the period length is 100 samples. According to the data, the first and the last 100 samples should have the same value. Fig. 1 shows the first and the last periods. It is clear from Fig. 1 that the periods do not coincide.

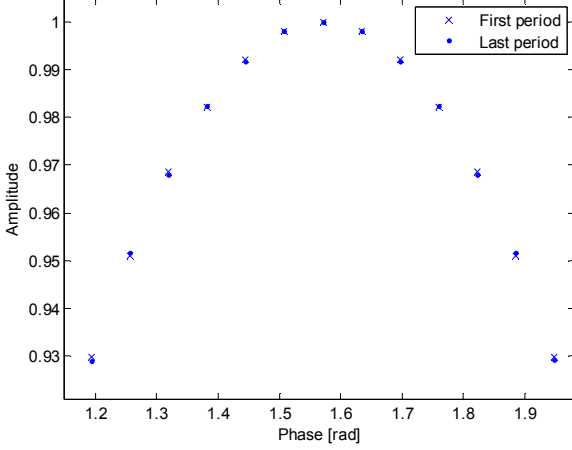


Fig. 1. Part of the first and the last periods of the evaluated sine wave

The problem is caused by the roundoff error of the phase evaluation, since the least significant bit $LSB(\varphi[n])$ increases with increasing n . For the first and the last samples:

$$LSB(\varphi[1]) = 7.45 \cdot 10^{-9}, LSB(\varphi[10^6]) = 3.9 \cdot 10^{-3}, \quad (6)$$

thus the error of the last sample is by 7 orders of magnitude higher, and similarly high is the evaluated value of the sine. Another problem is that $\frac{f_1}{f_s}$ is stored imprecisely even in this simple case. Here the value is 0.01 which has infinitely many bits in binary representation. The roundoff error is $2.23 \cdot 10^{-10}$. For the last sample of the record this introduces an error of $1.4 \cdot 10^{-3}$, which is lower than the error in (6) hence in Fig. 1 the noise-like error dominates. However, it has to be mentioned that the latter error is systematic, while the one introduced by rounding is noise-like. As a comparison to the values, the LSB of a 12-bit ADC is only $2.44 \cdot 10^{-4}$, so the error caused by the erroneous phase evaluation is much higher than the quantization error introduced by the ADC.

Calculating the phase like described in (5) results in a growing roundoff error with growing n , while the true phase information is always between $-\pi$ and π , since values of the sine and the cosine functions depend on the fraction of the phase only, taken with respect to 2π . However, by evaluating the phase with double precision and casting it back to single does not completely solve the problem, since the information is just in the fractional part which is again erroneous in single precision. To obtain a good value of the fractional phase, it

would be necessary to precisely calculate the phase, and precisely subtract the multiples of 2π .

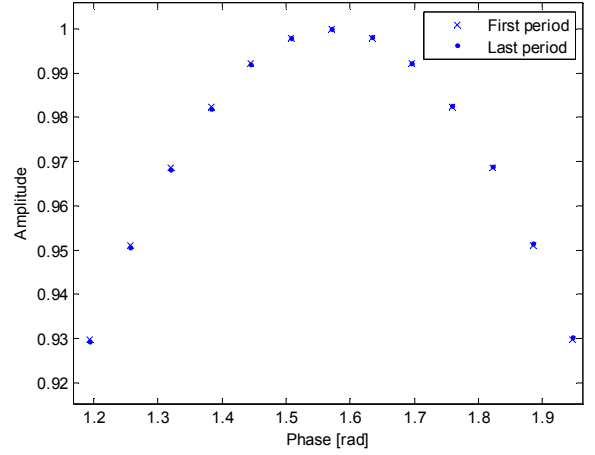


Fig. 2. Results of enhanced precision phase evaluation

A sophisticated (and suggested) solution is to calculate the fraction of $\frac{f_1}{f_s} n$, and multiply only this fraction by 2π . Fig. 2 shows the result of this modification. This method eliminates the noise-like error in (6) but does not eliminate the systematic error. For the errors see Fig. 3. It is apparent that the frequency information should be stored with enhanced precision, too.

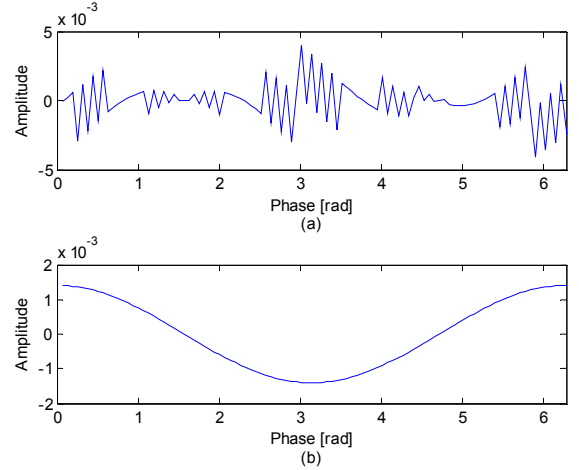


Fig. 3. Difference between the periods using (a) single precision and (b) enhanced phase evaluation

III. ROUND OFF ERROR IN THE SINE WAVE FIT ALGORITHMS

The roundoff error mentioned in Section II plays a major role in ALL sine wave fitting algorithms. In this section it is shown that each of the investigated algorithms suffers from the effect of different errors.

A. The effect of the phase evaluation error

The effect of the phase evaluation error is illustrated via the Three-Parameter LS method. In this case, the solution can be given in closed form [1] as:

$$\hat{s}_0 = (D_0^T D_0)^{-1} (D_0^T x), \quad (7)$$

where

$$D_0 = \begin{bmatrix} \cos(2\pi f_0 t_1) & \sin(2\pi f_0 t_1) & 1 \\ \cos(2\pi f_0 t_2) & \sin(2\pi f_0 t_2) & 1 \\ \vdots & \vdots & \vdots \\ \cos(2\pi f_0 t_N) & \sin(2\pi f_0 t_N) & 1 \end{bmatrix}, \quad (8)$$

\hat{s}_0 contains the estimated amplitudes of the in-phase and quadrature components of the signal model, and the unit offset i.e. A , B and C in (1), respectively and $t_n = \frac{n}{f_s}$. Finally \mathbf{x} is the digitized sample set [1].

The algorithm was evaluated for two sample sets from real measurements, each consisting of 100,000 samples. The signal frequency is 97 Hz, while the sampling frequency is 100 kHz. The nominal bit number of the ADC is 16. During the first experiment the ADC was driven to its full scale while for the second one it was overdriven so the fit was executed only for the samples in the operating range (approx. 65,000 samples). We assumed that the frequency is known with single precision.

TABLE I. ENOB OF THE CONVERTER FOR 100,000 SAMPLES

Sample set	ENOB values		
	Double precision	Single precision	Single precision with enhanced phase evaluation
1	12.4136	12.4118	12.4136
2 (overdriven)	12.3757	12.3675	12.3756

TABLE I. shows that there is no significant difference between the double precision and the single precision representations. However, if the sample number increases to 1 million, the results may be much more distorted. In TABLE II. it can be seen that for enhanced phase evaluation results are really close to each other, but without the enhancement, the value of *ENOB* decreases considerably.

TABLE II. ENOB OF THE CONVERTER FOR 1 MILLION SAMPLES

Sample set	ENOB values		
	Double precision	Single precision	Single precision with enhanced phase evaluation
1	12.3367	12.1376	12.3201
2 (overdriven)	12.1784	11.8180	12.1778

As it can be expected, the longer is the sample set, the larger is the effect of the roundoff error. For 1 million samples, the simple single-precision representation is significantly distorted.

It has to be mentioned that in this case only the phase evaluation was performed with increased precision, so we did not implement double representation on a single precision DSP. Each other method was performed with the original single precision.

B. Summation

Another problem that may occur during the CF evaluation (in the LS method the CF is the RMS value) is the summation

error. Let us consider an ideal quantizer, and an ideal noiseless sine wave as input, so that we only have input quantization error, and roundoff error. It was shown in [4] that the quantization error can be treated as a uniformly distributed variable between $-\Delta/2$ and $+\Delta/2$, and the expected value of the square of it is $\Delta^2/12$. Since the squared value is non-negative, the sum is growing, and the expected value of the sum in (2) is

$$E\{\sum_{n=1}^N (x[n] - y[n])^2\} = N \frac{\Delta^2}{12} \quad (9)$$

where Δ is the input quantum size. The variance of each error sample is $\frac{\Delta^4}{80}$, that of the sum is $N \cdot \frac{\Delta^4}{80}$. The relative std is $\frac{\sqrt{N \cdot \frac{\Delta^4}{80}}}{N \frac{\Delta^2}{12}} \approx \frac{1.34}{\sqrt{N}}$ which disappears for large N [4]. Since for the roundoff error LSB changes (increases) in each step, thus (9) cannot be applied. For floating-point, the relative errors are all equal, thus with linearly increasing sum the errors also grows linearly. (This is why even a modification of subtracting the approximate mean value helps, see Section IV). If the sum starts from $\Delta^2/12$ and grows linearly with the number of samples, the resulting relative roundoff error is significantly larger than the number representation error even for $N > 100$, thus it needs to be improved (see Section IV).

A possible solution is performing the summation with increased precision, but it slows down the algorithm considerably. Another way is using advanced summation techniques, keeping the single number representation (see Section IV).

C. Scaling

In many cases the frequency of the input data is not known. This parameter can also be estimated and the LS algorithm can be evaluated with four parameters. In this case, the method becomes iterative, calculating also the needed frequency correction (Δf) in each step, and a fourth column is also added to matrix D_0 .

$$D_0(x, 4) = \begin{bmatrix} -At_1 \sin(2\pi f_0 t_1) + Bt_1 \cos(2\pi f_0 t_1) \\ -At_1 \sin(2\pi f_0 t_2) + Bt_1 \cos(2\pi f_0 t_2) \\ \vdots \\ -At_1 \sin(2\pi f_0 t_N) + Bt_1 \cos(2\pi f_0 t_N) \end{bmatrix} \quad (10)$$

Adding the fourth parameter, however, includes a scaling problem, since the dimension of the frequency is different from that of the other three parameters and the condition number of matrix D_0 strongly depends on the scaling of the last column. In [5] the scaling of D_0 was also investigated, and it was frequency and record length dependent.

Scaling becomes of crucial importance using single precision, again. For ill-conditioned matrices even the pseudo-inverse of D_0 cannot be determined with required precision, hence the algorithm may diverge. For double precision numbers this error does not occur in reasonable cases, since roundoff errors are significantly lower.

In the following sections some additional error sources are described from which the Maximum Likelihood [2] and Quantile Based Estimator [3] methods suffer.

D. PDF of the Noise

The *Maximum Likelihood (ML)* method [2] tries to find the sine wave which is the most likely, given on a data set and assuming a known distribution for the (random) errors. Mathematically the method fits a sine wave, so that the log-likelihood function

$$\ln L(\mathbf{p}) = \sum_{k=1}^N \ln [P(Y(k) = y(k))] \quad (11)$$

is maximal, where $P(Y(k) = m)$ is the probability that the k^{th} sample of the random variable vector Y equals the digital code m , \mathbf{p} is the parameter set to be optimized, $y(k)$ is the k^{th} element of the digital sample set and N is the number of samples [2].

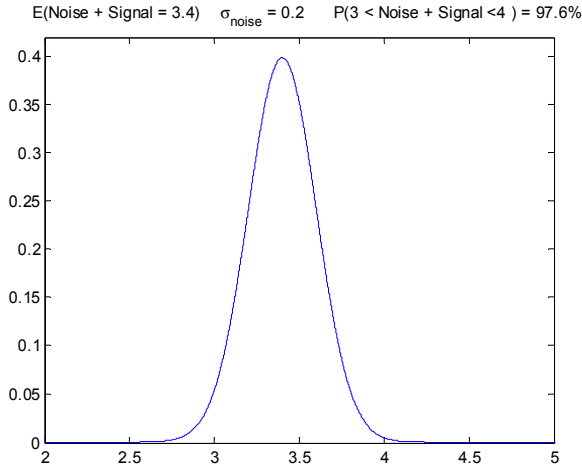


Fig. 4. Probability density function of the signal and the noise for a given sample

This method searches for the optimal solution in a five dimensional parameter space, also taking the additional noise into consideration which is mostly assumed to be Gaussian. The model is

$$x[n] = Q \left(A \cdot \cos \left(2\pi \frac{f_1}{f_s} n \right) + B \cdot \sin \left(2\pi \frac{f_1}{f_s} n \right) + C + \xi[n] \right), \quad (12)$$

where Q denotes the operation of quantization and $\xi[n]$ is the noise added to the n^{th} sample. Again, n varies from 1 to N .

The model of the noise determines the probabilities in (11). Fig. 4 illustrates the effect of the additive noise. Let us assume that we have an ADC with transition levels at integer numbers and for a given parameter set the k^{th} value of the fitted sine wave is 3.4. Furthermore, the noise is of Gaussian distribution with zero mean and $\sigma=0.2$. If in our measurement record the k^{th} sample is in the code bin between 3 and 4, then we can say that the probability of this measurement, using the given parameter set is 97.6%. This probability is to be calculated for each sample, and their logarithms are to be summed. The parameter set is searched, for which this sum is the highest.

It was shown in [7] that the bottom of the evaluated ML cost function is fairly ragged even for double number representation, thus good minimization can be difficult (close to the minimum the evaluated CF shows local minima). With 75-bit mantissa phase evaluation, however, the calculated cost

function is more or less smooth. The reason for the raggedness of the cost function is the roundoff error during evaluation.

Since this algorithm also tries to fit a sine wave, the roundoff error of phase evaluation mentioned in Section II also occurs – and similarly it will affect the probabilities at the end of the sample set.

Besides the phase evaluation error, other problems are also to be solved, when changing to single precision. One of these is caused by the probability density function (PDF) of the normal distribution. We think that the concrete shape of the PDF near the center is not very important: it is enough if it is Gaussian-like. However, if the Gaussian noise is an imperfect model for the tails, then the probability of an actually measured value, being somewhat off the signal model during iteration, may be very close zero (see below).

During the calculations it is assumed that the noise added to the measured signal is Gaussian. The probability that a random variable is between two values can be determined from the cumulative distribution function (CDF). In case of Gaussian random variables, the complementary error function (erfc) can be utilized for this purpose. However, the highest representable operand value for the CDF (for which the result can be distinguished from 1) is about 5.89σ for double and 3.91σ for single precision number representation. The problem is that for real measurements even values $|x - \text{signal}| > 5.89\sigma$ may occur, and if the differences are calculated between two points that are far from the mean value, the calculated probability is exactly 0, while under real circumstances, the probability is not 0 at all. On the other hand, it is also possible that for single representation, the result is exactly 0, while for double representation it differs from it. However, calculating the logarithm of 0 results in an infinite value of the log cost function, and the derivatives cannot be determined in this case, either. Therefore, $\log(CDF(x_2) - CDF(x_1))$ needs to be calculated directly.

The problem can be relaxed considering that also for real measurements higher noise values are sometimes present. A solution for this is to keep σ artificially high at least for a part of the iteration.

E. Stop criterion for Iteration

Iterative solutions (four-parameter method, maximum likelihood) can be sensitive to the above described problems, especially to raggedness of the CF.

i) Minimization methods which only use evaluated values of the CF (Nelder-Mead or simplex downhill, differential evolution, or fitting a quadratic form to a set of points close to the minimum) directly suffer from roundoff errors, and clearly prone to get stuck at (phantom) local minima. Periodic restarting with a blown-up starting set, or random perturbations of the parameter values can often help.

ii) Gradient-based methods

Our observation is that the evaluated value of the gradient is less sensitive to roundoff than the CF itself, thus gradient-based methods should perform better. Moreover, the function to be minimized is usually convex near to the minimum (the

Hessian is positive definite), and thus roundoff errors do not destroy the Hessian.

However, improved methods which avoid divergence especially further away from the minimum (e.g. Levenberg-Marquard, or simple observation of the decrease of the CF) pose an additional threat. Imprecise evaluation of the CF can hinder otherwise reasonable minimization steps, and unnecessarily decrease the step size applied. Thus even not at the minimum it is easy to think that there is no way to significantly decrease the CF. Thus, extra measures are necessary to avoid these situations.

F. Quantile Based Estimator

The Quantile Based Estimator [3] can be used primarily for the estimation of a constant, buried in noise, maybe disturbed by a sine, and measured with a known quantizer. It is based on the Gauss-Markov Theorem. It was shown that it approximates the ML estimate, while it is possible to calculate it very efficiently. This algorithm fits to the measured data

- i) either one parameter (constant C),
- ii) or three parameters (A, B, C or A_s, ϕ_s, C). In this case sampling needs to be coherent, and phases of the sinusoidal stimulus can assume only R distinct values [9] (that is, N/R is integer, equals the number of periods).

By assuming that accurate timing information is available, the collected samples can be grouped on a “per-phase” basis, and the three-parameter estimation using a sinusoidal stimulus can be transformed into an equivalent set of R estimation problems, each of them based on the usage of the constant stimulus at the ADC input, that in absence of noise is

$$d_r = C + A \sin(\phi_r), \quad r = 0, \dots, R-1, \quad (13)$$

where C is the sinewave offset, and ϕ_r is the r -th phase. By linearizing the effect of the noise on the CDF of the samples, an approximation of the Best Linear Unbiased Estimator (BLUE) can be derived, by using the conventional Gauss-Markov equation [8].

Generally in this method, the conventional Gauss-Markov estimate is calculated:

$$\hat{\theta} = (H^T \Sigma_W^{-1} H)^{-1} H^T \Sigma_W^{-1} X, \quad (14)$$

where Σ_W is the covariance matrix with $W[n] = X[n] - H[n]\theta$, X contains chosen rows of the data set, while H contains the chosen rows of (8).

By observing that quantized data is distributed according to a multinomial distribution, Σ_W can be estimated [8]. In fact, Σ_W has entries whose value depends on the probability of occurrence of each datum in the corresponding quantization bin. Thus, by counting the occurrences of data in each bin, the corresponding probability can be approximated and the covariance matrix can be estimated.

The Quantile Based Estimator, similarly to the ML estimator, can perform better than conventional estimators (e.g. sample mean) when estimating C , being able to remove the bias of the estimation (QBE is approximate ML, and ML is asymptotically unbiased).

Its advantage compared to the ML method is that when the above conditions of its usability are fulfilled, it provides an

estimate in just one step, similarly to the Three-Parameter LS fit. However, QBE in its present form can only estimate A, B, C , but not the fourth parameter, the frequency.

Since this estimator uses the fact that N/R is integer, it is not affected by the phase evaluation error as are the other ones, while it is sensitive to the assumed excellent synchronization of the periods. In other words, QBE tacitly assumes perfect knowledge of the phase values for the three-parameter case. Neither simulation nor measurement can provide exact values, thus numerical investigations are prone to roundoff.

Simulations showed that the QBE method is sensitive to frequency errors. Assuming that the frequency is known with a relative error of 10^{-7} the average ENOB was evaluated for 10 noisy stimuli. TABLE III contains the results which show that with increasing record length the ENOB decreases considerably.

TABLE III. – AVERAGE ENOB OBTAINED FOR $v_f=10^{-7}$

N	Average ENOB
10^6	7.69
10^5	11.06
10^4	13.00

Thus, while the problem highlighted in Section II is apparently greatly reduced in the case of the quantile based estimator, as few samples of the reference sine and cosine waves are needed in the observation matrix $H[n]$, the imprecision of synchronization (the limited knowledge of f_0/f_s , and its imprecisely integer value in reality) causes errors which are specific for QBE. Since the observation matrix contains a much lower number of entries than in the case of a conventional sine fit algorithm, the roundoff error problem associated to the calculation of (14) is somewhat less important.

IV. INCREASED PRECISION ON A GIVEN PLATFORM

In Section II it was mentioned that the phase can be evaluated with increased precision. It is a simple task on a PC for single precision, because hardware-supported double precision is also within reach. However, for single precision DSPs this solution cannot be chosen. In order to evaluate the phase with increased precision, we need to evaluate $n \frac{f_1}{f_s}$ with small error, and take the fractional part, and multiply by 2π . That means we need to implement at least multiplication (and sometimes also the addition) operations with enhanced precision.

To be able to do that, first we have to find a representation that enables increased bit number representation while not slowing down the computer too much. E.g. for double representation the number can be split into three parts, each containing 25 bits (double precision representation has 53-bit mantissa). The difference between the exponents is always 25 in this case, see Fig. 5.

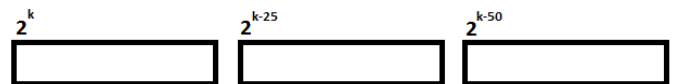


Fig. 5. Enhanced precision number representation

Calculating the multiplication can be based on convolution, see Fig. 6.

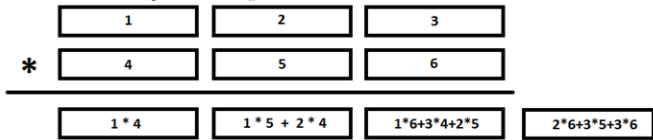


Fig. 6. Multiplication with enhanced precision number representation

The addition operation can also be simply calculated. First, the numbers have to be shifted so that the exponents of the most significant parts are equal to each other. Then the addition can be executed.

It is critical that overflow must be treated. That means that e.g. if $2+5$ cannot be represented on 25 bits any more, the overflow is to be added to the first term of the sum, etc.

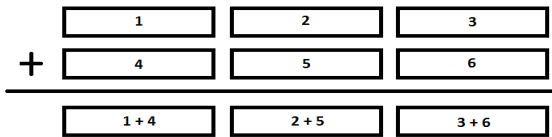


Fig. 7. Addition with enhanced precision number representation

It is important to mention two things here.

i) During the evaluation of the sine fitting algorithms only the phase needs to be calculated with enhanced precision.

ii) Precision enhancement as described above has practical relevance only if we do not implement an increased precision evaluation on a restricted precision platform, e.g. double precision on a single precision platform. Namely, in theory any required precision can be reached like that but the algorithms cannot be run with a reasonable time limit.

For the summation, Section III. B shows that the roundoff error of summation is much larger than the number representation error. This can cause a noticeable raggedness at the bottom of the CF. If this needs to be decreased, the above method can also be used, but also rather simple but much quicker improved-precision summation techniques can be utilized, like

a) Subtraction of the approximate mean value of each number, and calculate the result as $\sum_{k=1}^N (x(k) - m) + N \cdot m$, where m denotes the mean value.

b) Dividing the numbers into groups and subgroups, like in the FFT, and add them pairwise, then pairwise, etc.

c) Maybe a combination of both (usually not necessary)

d) Applying the so-called Kahan-compensation [6]. This method stores the roundoff error after each summation step and compensates for it, this way increasing the precision artificially. For example let us assume that after many summation steps the sum equals to 10^6 and the next element is 0.2. The algorithm adds this two numbers, subtracts 10^6 and then 0.2. The result is $-4.64 \cdot 10^{-10}$ and that is the roundoff error. This error is added to the next term, this way compensating the error of the previous addition, etc.

V. CONCLUSIONS

In this paper numerical problems of sine wave fit algorithms were investigated. It was shown that due to calculation errors different algorithms yield imprecise results. The source of these errors can be phase evaluation error, summation error, scaling problem, or imprecise noise CDF evaluation and have an effect especially for single representation and long records. The error comes up for Three- and Four-Parameter Sine Wave Fit, for the Maximum Likelihood method and also for the Quantile Based Estimator, and can be significantly reduced by the given techniques. For all methods precise phase evaluation, for the Four-parameter LS fit a scaling, for the ML fit a relaxing method was suggested in order to improve numerical performance. Finally, a possible solution was given to artificially increase precision on a given platform.

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