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Improving the Conditioning of Maximum Likelihood Sine Wave Fitting

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***Abstract* – In this paper, a scaling method is proposed and studied for the maximum likelihood sine fitting algorithm. It is shown that similarly to the case of least squares fitting, this method can significantly improve the conditioning of the investigated algorithm. The maximum error in the solution of a linear system of equations strongly depends on the condition number of the coefficient matrix. Namely, the condition number of the coefficient matrix upper bounds the relative error of the solution. It is shown that the condition number of the maximum likelihood fitting is connected to the Hessian matrix. Thus, this matrix is analyzed to find general properties increasing the condition number. It is pointed out that the scaling factor applied for the least squares fitting also decreases the conditioning of the Hessian matrix significantly. By this means, the numerical stability of the maximum likelihood fitting is improved. Theoretical results are verified through simulations.**

***Keywords* – Signal processing, maximum likelihood estimation, sine fitting, condition number, numerical accuracy**

I. INTRODUCTION

Estimation of the parameters of a sine wave is a common task in measurement technology: the problem arises in analog-to-digital converter (ADC) testing, harmonic analysis of power networks, system identification and in many other fields of electrical engineering.

Literature provides several algorithms to solve this problem. They differ in complexity, precision, accuracy and computational demand. One of the most commonly used methods is the time domain least squares (LS) fitting, defined in IEEE Standard 1241 [1]. In this algorithm, the parameters are adjusted so that the sum of squared differences between the fitted and measured sine waves is minimal. The method implicitly assumes uniform and ideal quantization. Once the sine is measured on a real ADC with non-zero integral nonlinearity (INL), results are getting distorted. A much more complex method is the maximum likelihood (ML) fitting [4] which can handle the above problem. In the ML algorithm, besides sine parameters, the standard deviation of the noise and transition levels of the ADC are also estimated. The most important advantages of the ML method are asymptotical unbiasedness and minimum variance among the estimation methods (which holds true even for non-ideal quantization).

A common point of LS and ML methods is their possible numerical instability: both algorithms require matrix inversion calculations which can be challenging for large number of samples and columns of largely different magnitudes.

The condition number (CN) is a good measure of stability. It is defined as the ratio of the largest and smallest singular values of a matrix [2]. Solving linear systems of equations with ill-conditioned coefficient matrices are likely to result in significant errors even with 64-bit double precision number representation, and might prevent the precise estimation of the sine parameters. In this paper, a scaling method is presented in order to handle the problem of ill-conditioning.

II. BACKGROUND AND NOTATION

A sine wave can be characterized by the following description:

$$y_k = R \cdot \cos(2\pi f t_k + \phi) + C, \qquad (1)$$

where y_k is the kth sample in the fitted sine wave, R, ϕ and C are the amplitude, initial phase and offset components, respectively, and f denotes the frequency of the signal. However, this model is not advantageous in optimization problems. Namely, it is nonlinear in two parameters (f, ϕ). Fortunately, the initial phase can be eliminated by using the following form:

$$y_k = A \cdot \cos(2\pi f t_k) + B \cdot \sin(2\pi f t_k) + C, \qquad (2)$$

where A and B are the cosinusoidal and sinusoidal components of the signal, respectively. The description can be given in another way, assuming that the sampling

is equidistant, that is:

$$t_k = \frac{k}{f_s} \ , \tag{3}$$

where f_s denotes the sampling frequency. In this case:

$$\begin{gathered} y_k = A \cdot \cos(k\vartheta) + B \cdot \sin(k\vartheta) + \mathrm{C} \\ \vartheta = 2\pi \frac{f}{f_s} \end{gathered} \tag{4}$$

where ϑ is the (to the sampling frequency) relative angular frequency.

To fit a sine wave, a fitting criterion is needed. In [1], a time domain least squares (LS) fitting is prescribed. For this fitting, a parameter set is searched that minimizes the squared differences between the fitted and sampled sine waves. The cost function (CF) of this fitting is:

$$\mathrm{CF_{LS}} = \sum_{k=1}^{N} (x_k - y_k)^2 \tag{5}$$

where *N* denotes the number of samples and x_k is the *k*th element in the sampled record.

If the frequency of the signal is known, a three-parameter fitting is needed. Otherwise, the frequency has to be estimated, as well. This turns the problem into non-linear, implying that an iterative optimization is required. A general and commonly used method in this case is the Gauss-Newton method, which is proposed in [1] (with minor modifications). The least squares solution in the *i*th step is calculated in the following form:

$$\begin{gathered} \mathbf{p} = \begin{pmatrix} A \\ B \\ C \\ \Delta\vartheta_i \end{pmatrix} , \\ \mathbf{D}_i \mathbf{p}_i = \boldsymbol{y} \ , \\ \widehat{\mathbf{p}}_i = \left(\mathbf{D}_i^{\mathbf{T}} \mathbf{D}_i\right)^{-1} \mathbf{D}_i^{\mathbf{T}} \boldsymbol{y} \ . \end{gathered} \tag{6}$$

where $\mathbf{p}$ denotes the parameter vector to be estimated and $\widehat{\mathbf{p}}_i$ is the estimator in the *i*th iteration. In the above equation, $\mathbf{D}_i$ is the coefficient matrix of the least-squares equation:

$$\mathbf{D}_i = \begin{pmatrix} \cos\vartheta & \sin\vartheta & 1 & D_{i,14} \\ \cos 2\vartheta & \sin 2\vartheta & 1 & D_{i,24} \\ \vdots & \vdots & \vdots & \vdots \\ \cos N\vartheta & \sin N\vartheta & 1 & D_{i,N4} \end{pmatrix} \tag{7}$$

$$D_{i,k4} = 2\pi k(-A_{i-1}\, sin\, k\vartheta + B_{i-1}\, cos\, k\vartheta)$$

The LS solution of the fitting can be obtained by calculating the Moore-Penrose pseudo inverse of $\mathbf{D}_i$. The simplest calculation method is:

$$\mathbf{D}_i^{+} = \left(\mathbf{D}_i^{\mathbf{T}} \mathbf{D}_i\right)^{-1} \mathbf{D}_i^{\mathbf{T}} \tag{8}$$

where $\mathbf{D}_i^{+}$ denotes the pseudo inverse of $\mathbf{D}_i$. However, from a numerical point of view, this evaluation is advantageous only if the CN of $\mathbf{D}_i$ is small. Namely, the larger the CN, the higher the sensitivity of the solution of the system of equations to small perturbations [2]. The CN of $\mathbf{D}_i^{\mathbf{T}} \mathbf{D}_i$ equals to the square of the CN of $\mathbf{D}_i$. Thus, evaluating the pseudo inverse of an ill-conditioned $\mathbf{D}_i$ according to (8) increases numerical instability. To avoid this problem, decomposition methods, like QR-decomposition or singular value decomposition (SVD) can be applied [2]. Nevertheless, decomposition methods only prevent the CN from being squared. Ill-conditioned problems remain ill-conditioned even if these methods are used. Thus, it is reasonable to investigate how the CN can be decreased.

In order to determine the CN of the LS problem, $\mathbf{D}_i^{\mathbf{T}} \mathbf{D}_i$ was investigated in [3] and [7]. It was pointed out that the following approximation holds:

$$\mathbf{D}_i^{\mathbf{T}} \mathbf{D}_i \approx \begin{pmatrix} \frac{1}{2} & 0 & 0 & \frac{BN}{4} \\ 0 & \frac{1}{2} & 0 & -\frac{AN}{4} \\ 0 & 0 & 1 & 0 \\ \frac{BN}{4} & -\frac{AN}{4} & 0 & \frac{R^2N^2}{6} \end{pmatrix} \tag{9}$$

In the ML method, the signal is assumed to be quantized by a (non-ideal) quantizer:

$$x_k = Q(y_k + \xi_k) \qquad n = 1 \ldots N \tag{10}$$

where $Q(\cdot)$ denotes the operation of quantization, and ξ_n is the additive noise that is mostly assumed to be of Gaussian distribution with zero-mean and standard deviation σ. In the ML estimation, a parameter set is searched that maximizes the probability of observing the sampled data set. Since a noise model is also added, the standard deviation of the additive noise is to be estimated, as well. The main advantage of the ML method is that the non-ideality of the quantizer is taken into account during the calculation of sine parameters. Thus, the estimation is (asymptotically) unbiased independently from the quantizer characteristics.

The probability that the *k*th sample is in code bin l equals

to [5]:

$$P(X_k = l) = \frac{1}{2}\left[\mathrm{erf}\left(\frac{T_l - y_k}{\sigma\sqrt{2}}\right) - \mathrm{erf}\left(\frac{T_{l-1} - y_k}{\sigma\sqrt{2}}\right)\right], \quad (11)$$

where T_l is the lth transition level. The CF of the ML estimation is [5]:

$$\mathrm{CF_{ML}} = -\sum_{n=1}^{N} ln[\mathrm{P}(X_k = x_k)] \ . \quad (12)$$

The negative sign is needed in order to turn the probability maximization problem into a minimization problem. The CF can be effectively minimized by the Levenberg-Marquardt algorithm [9]. This method is implemented in the ADC toolbox [6]. In the Levenberg-Marquardt algorithm, the fine tuning of the parameters can be determined by:

$$\Delta\mathbf{p} = -\left(\frac{\partial^2 \mathrm{CF}(\mathbf{p})}{\partial\mathbf{p}^\mathbf{T}\partial\mathbf{p}} + \lambda\mathbf{I}\right)^{-1} \frac{\partial \mathrm{CF}(\mathbf{p})}{\partial\mathbf{p}} \quad (13)$$

where λ is set during the optimization, $\frac{\partial \mathrm{CF}(\mathbf{p})}{\partial\mathbf{p}}$ is the gradient of the cost function, and $\frac{\partial^2 \mathrm{CF}(\mathbf{p})}{\partial\mathbf{p}^\mathbf{T}\partial\mathbf{p}}$ is the Hessian matrix of the cost function. If $\lambda \to \infty$, the method becomes a step in the direction of the gradient, while with $\lambda = 0$, we get the Newton-Raphson method. This latter method can find the optimum of a quadratic CF in one step. In the vicinity of the optimum, the CF can be assumed to be quadratic, so the value of λ can be decreased. With $\lambda = 0$, we obtain:

$$\Delta\mathbf{p} = -\left(\frac{\partial^2 \mathrm{CF}(\mathbf{p})}{\partial\mathbf{p}^\mathbf{T}\partial\mathbf{p}}\right)^{-1} \frac{\partial \mathrm{CF}(\mathbf{p})}{\partial\mathbf{p}} \ . \quad (14)$$

It is obvious that the conditioning of this problem is connected to the CN of $\frac{\partial^2 \mathrm{CF}(\mathbf{p})}{\partial\mathbf{p}^\mathbf{T}\partial\mathbf{p}}$, that is, to the Hessian matrix of the CF.

III. RELATED RESULTS IN THE LITERATURE

In this section, results on the conditioning of the four-parameter least squares method will be summarized. In [3] and [7], it was pointed out that the condition number of the LS method can be significantly decreased, if the fourth parameter is scaled (the fourth column in $\mathbf{D}_i$ is divided by a scaling factor):

$$\left(\mathbf{D}_i^\mathbf{T}\mathbf{D}_i\right)_{\mathrm{scaled}} \approx \begin{pmatrix} \frac{1}{2} & 0 & 0 & \frac{BN}{4\gamma} \\ 0 & \frac{1}{2} & 0 & -\frac{AN}{4\gamma} \\ 0 & 0 & 1 & 0 \\ \frac{BN}{4\gamma} & -\frac{AN}{4\gamma} & 0 & \frac{R^2N^2}{6\gamma^2} \end{pmatrix} \quad (15)$$

where γ denotes the scaling factor. The optimal scaling γ_{opt} was shown to be [7]:

$$\gamma_{\mathrm{opt}} = \frac{RN}{1.852} \ . \quad (16)$$

In [7], a Monte Carlo analysis was carried out in order to demonstrate the effectiveness of the scaling. The analysis showed that with the proposed scaling, the CN of the scaled $\mathbf{D}_i^\mathbf{T}\mathbf{D}_i$ does not exceed 20, provided that at least 4 periods are sampled from the signal and at least four samples are sampled from one period. If the number of sampled periods is increased above 100, the condition number drops under 15.

IV. DESCRIPTION OF THE METHOD

During the LS estimation, matrix $\mathbf{D}_i$ contains the derivatives of the fitted signal. Notice that $\mathbf{D}_i^\mathbf{T}\mathbf{D}_i$ is connected to the Hessian matrix of the LS fitting, since [10]:

$$\frac{\partial^2 \mathrm{CF_{LS}}(\mathbf{p})}{\partial\mathbf{p}^\mathbf{T}\partial\mathbf{p}} \approx 2\left(\frac{\partial\boldsymbol{y}}{\partial\mathbf{p}}\right)^\mathrm{T}\left(\frac{\partial\boldsymbol{y}}{\partial\mathbf{p}}\right) = 2\mathbf{D}_i^\mathbf{T}\mathbf{D}_i \ . \quad (17)$$

It is known that in case the additive noise is white, of Gaussian distribution and zero-mean, the ML and LS estimates coincide [8]. Thus, it is reasonable to use the same scaling for the ML estimation, as for the LS estimation to ensure the good-conditioning of the Hessian matrix in (13).

In order to represent this, let us analize the second derivative of $\mathrm{CF_{ML}}$ with respect to the relative angular frequency:

$$\frac{\partial^2 \mathrm{CF_{ML}}(\mathbf{p})}{\partial\vartheta^2} = \sum_{\mathrm{k}=1}^{N} \frac{1}{\alpha_k^2}\left(\frac{\partial\alpha_k}{\partial\vartheta}\right)^2 - \frac{1}{\alpha_k}\frac{\partial^2\alpha_k}{\partial\vartheta^2} \ . \quad (18)$$

where α_k is the argument of the natural logarithm function in (12), that is

$$\alpha_k = \mathrm{P}(X_k = x_k) \ . \quad (19)$$

First, let us investigate the value of $\partial\alpha_k/\partial\vartheta$:

$$\frac{\partial \alpha_k}{\partial \vartheta} = \frac{2}{\sqrt{\pi}} \cdot \frac{A\sin(k\vartheta) - B\cos(k\vartheta)}{\sqrt{2}\sigma} k \cdot \left(e^{-\left(\frac{\mathrm{T}[y_k+1]-x_k}{\sqrt{2}\sigma}\right)} - e^{-\left(\frac{\mathrm{T}[y_k]-x_k}{\sqrt{2}\sigma}\right)} \right), \quad (20)$$

It can be seen that the result grows with growing k. Furthermore, it is proportional to the amplitude of the signal (R). It can be shown similarly that $\partial^2\alpha_k/\partial\vartheta^2$ is also proportional to these values. Thus, $\frac{\partial^2 \mathrm{CF_{ML}}(\mathbf{p})}{\partial \vartheta^2}$ increases with increasing N and R. However, its value cannot be approximated as easily as for the case of the LS method. Namely, the ML method takes quantizer non-linearities into consideration. Thus, the problem cannot be solved generally. Nevertheless, we can expect significant improvement in the conditioning of the Hessian matrix, if it is scaled with a proper scaling factor.

The Maximum Likelihood method optimizes the parameters iteratively to maximize the Likelihood function. The update step (as described in Section II) is the following:

$$\Delta\mathbf{p} = -(\mathbf{H} + \lambda\mathbf{I})^{-1} \frac{\partial \mathrm{CF}(\mathbf{p})}{\partial \mathbf{p}} \quad (21)$$

where **H** is the Hessian matrix, which contains the second order derivatives of the cost function (thus it is positive-definite):

$$\mathrm{H_{ij}} = \frac{\partial \mathrm{CF}(\mathbf{p})}{\partial \mathrm{p}_i \partial \mathrm{p}_j} \quad (22)$$

In the above equation, **p** is the vector of the estimated parameters:

$$\mathbf{p} = \begin{pmatrix} A \\ B \\ C \\ f \\ \sigma \end{pmatrix} \quad (23)$$

Equation (21) shows that the numerical stability of the calculation of the new set of parameters strongly depends on the CN of the Hessian matrix: if it is ill-conditioned, significant errors might appear in the calculation, resulting in numerical instability and distorted estimation of the parameters. To avoid such errors, the following weighing matrix was used to improve numerical performance:

$$\mathbf{W} = \mathrm{diag}\langle 1\ 1\ 1\ \frac{1}{\gamma_{\mathrm{opt}}}\ 1\rangle . \quad (24)$$

The value of γ_{opt} is calculated according to (16). The scaled Hessian matrix is determined by:

$$\mathbf{H}' = \mathbf{W}^{\mathbf{T}}\mathbf{H}\mathbf{W} . \quad (25)$$

By this means, the fourth parameter, that is, ϑ is scaled similarly to the case of LS fitting

V. RESULTS AND DISCUSSIONS

The proposed algorithm was tested in simulations where the condition numbers of the scaled and the original Hessian matrix were compared. In the simulations, a 14-bit ADC was applied with INL and DNL characteristics that are depicted in Figures 1 and 2.

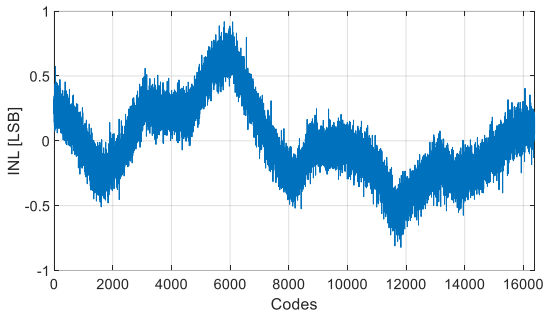

Figure 1. INL of the 14 bit ADC

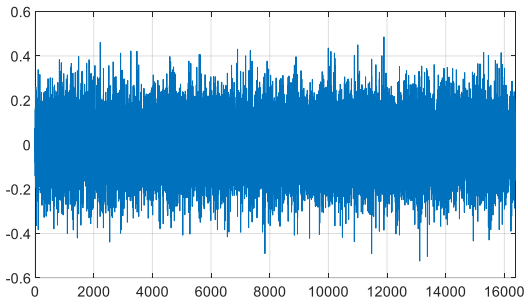

Figure 2. DNL of the 14 bit ADC

The ADC was excited with a sine wave input:

$$x_k = R \cdot \cos\left(2\pi \frac{J}{N} k + \phi\right) + C . \quad (26)$$

where J is the number of sampled periods. 100 different cases were studied with $N = 2^{18}$, $R = 2^{13}$ LSB (least significant bit) and C=0. The further parameters of the sine were the following random variables:

- J was uniformly distributed in the [5, 65536] domain
- ϕ was uniformly distributed in the [0, 2π] domain.

In addition, to simulate real-like circumstances, Gaussian noise with 1 LSB standard deviation and harmonic distortion at frequency $2J$ with 1 LSB amplitude and

random initial phase ϕ_h was added to the sinewave before quantization:

$$h_k = LSB \cdot \cos\left(4\pi \frac{J}{N} \mathrm{k} + \phi_h\right). \qquad (27)$$

$$z_k = N(0, LSB). \qquad (28)$$

where $N(0, LSB)$ denotes Gaussian distribution with zero-mean and 1 LSB standard deviation. Quantized signal $\mathbf{x}_Q$ can be obtained by:

$$\mathbf{x}_Q = Q(\mathbf{x} + \mathbf{z} + \mathbf{h}). \qquad (29)$$

The ML method requires an initial estimation of the signal parameters and the quantizer characteristics. Thus, first a histogram test was performed to estimate the transition levels of the ADC. Then, the parameters of the input signal were estimated using the LS method.

In the simulations, the estimation was run with both scaled and unscaled Hessian matrix, and the condition numbers in both cases were determined. In the scaled case, the Hessian matrix was calculated according to (25). Condition numbers in both cases can be seen in Figures 3 and 4.

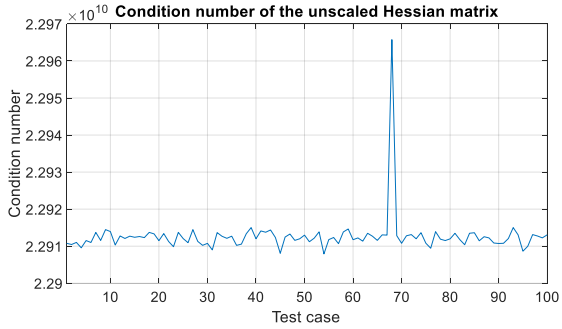

Figure 3. Condition number of the unscaled Hessian matrix

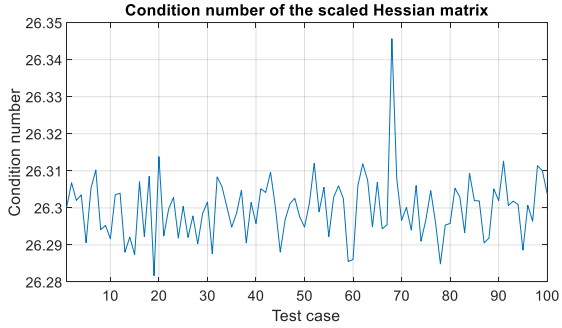

Figure 4. Condition number of the scaled Hessian matrix

The figures show that the proposed method reduced the CN significantly. The values in the scaled cases are 10^9 times smaller than the original ones, ensuring good-conditioning (the CNs do not exceed 30). As a result, the numerical stability of the matrix inversion in (21) was significantly increased. Since the error in the resulting parameter vector depends linearly on the condition number of the Hessian matrix (see [2]), the possible distortions in the estimator are much more limited to a smaller extent.

VI. CONCLUSIONS

In this paper, a scaling method for the Hessian matrix of the maximum likelihood fitting was presented. It was shown that the same scaling factor can be applied that improves the conditioning of the least squares fitting. Simulation results showed that the presented scaling algorithm considerably reduces the condition number of the Hessian matrix: in the studied cases, the condition number was found to be 10^9 times smaller than its original value. This enhancement ensures that the inversion of the Hessian matrix can be evaluated in a numerically stable way. Thus, the numerical accuracy of the maximum likelihood method was shown to be improved significantly.

VII. ACKNOWLEDGMENT

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