An Efficient Nonlinear Least Square Multisine Fitting Algorithm

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***Abstract*—This paper presents a new nonlinear least-squares algorithm for fitting band-limited periodic signals with unknown frequency and harmonic content. The new solution features a model-based recursive calculation method that requires less memory space and has smaller computational demand than the known matrix-based algorithms.**

***Index Terms*—Least squares methods, parameter estimation, periodic functions, recursive estimation, resonator filters.**

I. Introduction

THE estimation of the harmonic content of periodic signals is a very common problem and the solution is also very well known for several typical scenarios. If the signal's frequency is known *a priori* and the record contains a whole number of periods, then the solution can be computed by the fast Fourier transformation (FFT). If the generator and the acquisition device are not synchronized, then a linear least-squares (LS) problem must be solved to gain the unknown amplitude values; in this case, the computational load is higher than in the synchronized case. If the signal frequency is not known either, then a much more complicated nonlinear least-squares (NLS) problem must be solved. In typical cases, when the record contains only a reasonable number of points and frequency lines to be estimated (up to a few thousand data points and a few hundred frequencies), the problem can be solved using the methods available in the literature [1]. Based upon this method, the solution of the NLS problem requires roughly $O(MN^2)$ operations and $O(MN$ storage space, where M represents the number of harmonics to be estimated, and N is the length of the time record. If the number of samples and/or the harmonics to be estimated exceeds a certain limit, these methods cannot be used in conventional computers any more because of the slowdown of these algorithms and, especially, of the extreme memory requirements. This paper presents a new model-based solution, which uses a tuned resonator-based filter bank [2]. The proposed method requires $O(MN)$ operations and $O(N)$ storage space. The low memory requirements and the recursive nature of the computation make the hardware implementation also possible.

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II. Nonlinear Least-Squares Algorithm

The classical parameter estimation problem of periodic signals with unknown frequency and amplitude content can be formulated as follows

$$s(k) = \sum_{m=-M}^{M} A_m e^{jkm\omega_0} \left(A_m = A_{-m}^*, k = 0, 1, \ldots, N-1\right) \tag{1}$$

where $s(k)$ is the estimate of the discrete-time periodic signal $s_m(k)$ at time instant k. The angular frequency is ω_0 and A_m is the complex amplitude of the mth harmonic. The frequency ω_0 and the harmonics amplitudes A_m are to be estimated in least-squares sense so that the squared error

$$E^2 = \sum_{k=0}^{N-1} e(k)^2 = \sum_{k=0}^{N-1} \left(s_m(k) - s(k)\right)^2 \tag{2}$$

is minimal. A well-formed solution was presented in [1]; the main features of the nonlinear least squares algorithm (NLS) are briefly described here.

Theoretically, the iterative solution of the NLS problem can be divided into two main parts. Part 1 is a solution of a linear LS problem with a fixed frequency value; then, in Part 2, a new frequency estimate is calculated using a Gauss-Newton gradient-search procedure. Then, Parts 1 and 2 are repeated until no improvement is achieved any more. The algorithm proposed in [1] performs the iterative steps without the explicit calculation of the linear LS solution (Part 1 is hidden in Part 2), thus providing numerically stable and fast calculation. Since the derivative $\partial E^2/\partial\omega_0$ can be calculated (see [1]), a Gauss-Newton procedure is used to find the minimum versus the fundamental frequency. Note that although the gradient search algorithm always finds a (local) minimum, it is necessary to have an initial guess of the frequency, which is sufficiently close to the true frequency value, in order to guarantee convergence to the global minimum (see the example in Section IV). The algorithm described in [1] uses matrix calculations and its numerically stable and effective implementation requires $O(NM)$ memory space and $O(NM^2)$ operations.

Identification algorithms require the sample mean and its variance as input quantities to provide parametric models on the signal or system [3]. The calculation of these quantities is usually performed as follows.

- The frequency value is estimated by solving the nonlinear LS problem.
- The data record is segmented into B separate (or only slightly overlapping) parts. The segments usually contain a full number of periods. If it is possible, B should be at least four [3].
- The linear LS problem is solved for each segment, thus providing B sets of Fourier coefficients.
- The sample mean is calculated by taking the mean value of the Fourier-coefficients over the B sets, after appropriate phase reconstruction.
- The sample variance is the variance of the B different (phase-reconstructed) representations. The variance of the sample mean is calculated as $1/B$ times the sample variance.

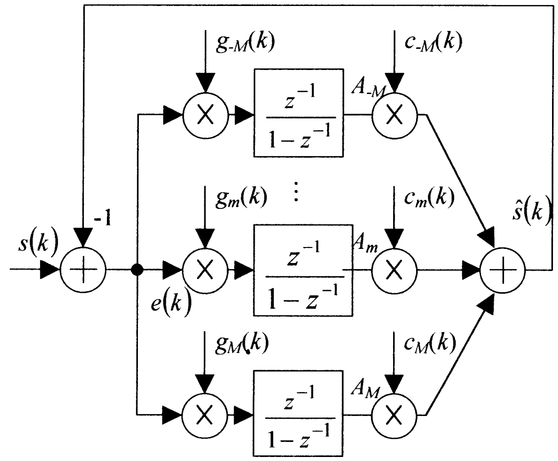

Fig. 1. Resonator-based observer.

III. Resonator-Based NLS Algorithm

A model-based structure was proposed in [2] for recursive discrete transforms, which was proven especially suitable for calculating the discrete Fourier transformation. The structure is nothing but an observer containing an embedded model of the signal to be measured, as shown in Fig. 1. If the signal model is the same as in (1), then the corresponding resonator-based structure has the following parameters

$$\left.\begin{array}{l} c_m(k) = e^{j\omega_0 mk} \\ g_m(k) = r_m e^{-j\omega_0 mk} \end{array}\right\} m = -M, \ldots, 0, \ldots, M, M\omega_0 < \pi \quad (3)$$

and A_m contains the Fourier coefficients for the mth harmonic ($A_m = A^*_{-m}$). The coefficients r_m can be used to set the pole placement of the structure. For a dead-beat observer, the parameters can be calculated as follows

$$r_m = \frac{1}{\prod_{\substack{i=-M \\ i\neq m}}^{M} (1 - z_i z_m)}, z_i = e^{j\omega_0 i}. \quad (4)$$

With these settings, the $A_m(k)$ outputs of the system contain the Fourier coefficients of the segment $[s(k-2M-1), \ldots, s(k-2), s(k-1)]$ after the initial transient of $2M+1$ samples.

Notes

- The resonator bank structure is able to compute the Fourier coefficients of the input signal in a sliding window manner (i.e., the new result is available at every time instant).
- The computation is synchronized to the fundamental frequency ω_0; so, leakage and picket fence effects can be avoided without synchronizing the sampling frequency.
- The computational complexity is $O(M)$ operation per sample, or $O(MN)$ operations for a block of length N.
- The memory requirement of the algorithm is $O(M)$ for the calculations, or $O(N)$ for a record of length N if the input must also be stored.

Using the resonator-based structure, a new algorithm has been constructed to solve the nonlinear least-squares problem for periodic signal parameter estimation. In the proposed method, the resonator bank structure is used to solve the linear LS problem (in Part 1, ω_0 is supposed to be known), with the settings (3)–(4). The iterative Part 2 (upgrade of the frequency estimator) would require $\partial E^2/\partial\omega_0$ in order to use a gradient method. Unfortunately, the derivative in this framework is not known, so another pseudo-gradient search must be used. The main features of the proposed search method are the following

- It is supposed that the error surface is a parabola (note that the same assumption is made using the Gauss-Newton method). This approximation is good if the frequency estimate is close to the true value (see the example in Section IV).
- Unlike in conventional gradient search methods, it is not the gradient value in one point that is used to find the bottom of the error surface, but rather a parabola is fitted to three different points to estimate the minimum point.

If the frequency estimate is close to the true value, the behavior of the proposed solution is very similar to that of the Gauss-Newton method. The reason is that both algorithms use the same model (quadratic error surface) built-in the search method. The only disadvantage of the newly proposed method is that three frequency points must initially be supplied to the algorithm, each of them sufficiently close to the true value, instead of one (see Figs. 2 and 3). The proposed algorithm works as follows.

Part 1 (The Linear LS Solution):

L1 Determine M and the signal model (3) from the frequency estimate ω_0. Note that if the number of frequency lines is not known *a priori*, M is the total possible number of frequencies (i.e., $[\pi f_s/\omega_0]$, where f_s is the sampling frequency).

L2 Calculate the values r_m using the current frequency estimate ω_0, according to (4).

L3 Run the resonator bank for the whole record of length N, using the appropriate signal model (3).

L4 Calculate the sample mean (see below).

L5 Compute the least-squares error according to (2).

Part 2 (NLS Iteration):

N1 An initial frequency value is selected together with two neighboring points.

N2 For all three frequency estimates calculate the linear LS solution (Part 1).

N3 A parabola is fitted to the three points in the frequency—LS error space and a new frequency estimate

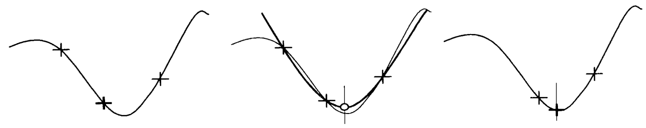

Fig. 2. The minimum search procedure. a) The error surface with three measurement points, the lowest being the current estimate of the minimum; b) the fitted parabola with its minimum; c) the new measurement points, the lowest is the updated estimator.

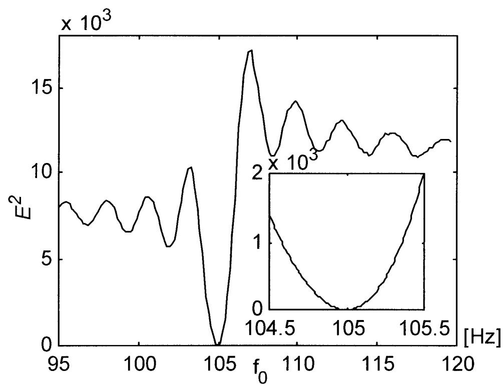

Fig. 3. Error surface versus the estimate of the fundamental frequency. The true value is $f_0 = 105$ Hz.

is calculated where the parabola is minimal. The frequency value farthest from the new frequency is replaced by the new frequency at the minimum (see Fig. 2).

N4 The linear LS solution (Part 1) is calculated for the new point, providing a new set of three points in the frequency—LS error space.

N5 Steps N3-N4 are repeated until the improvement is below a limit.

N6 Calculate the sample variance (see below).

The calculation of the sample mean is quite straightforward (the calculated Fourier coefficients are in-phase, so no further phase reconstruction is required) and can be made in two different ways.

If the record contains several periods, then the conventional block-wise calculation can be used. If there are B blocks of length $L = 2M + 1$ ($N \cong BL$), then the sample mean of a Fourier coefficient A_m is

$$\bar{A}_m = \frac{1}{B}\sum_{b=1}^{B} A_m(Lb) \tag{5}$$

and the sample variance is calculated by

$$\hat{\sigma}^2(A_m) = \frac{1}{B-1}\sum_{b=1}^{B}\left|\bar{A}_m - A_m(Lb)\right|^2 \tag{6}$$

from which the sample variance of the sample mean can be calculated as follows:

$$\hat{\sigma}^2(\bar{A}_m) = \frac{1}{B}\hat{\sigma}^2(A_m). \tag{7}$$

If the record is short and no separate segments can be constructed (but the record contains at least M samples, which means at least one full period if all the possible harmonics are used), then all of the $A_m(k)$ estimates, which are available at each time instant, can be used to calculate the sample mean and the sample variance

$$\bar{A}_m = \frac{1}{N-L}\sum_{k=L}^{N-1} A_m(k), \tag{8}$$

$$\hat{\sigma}^2(A_m) = \frac{1}{N-L-1}\sum_{k=L}^{N-1}\left|\bar{A}_m - A_m(k)\right|^2. \tag{9}$$

Because of the strong correlation of the samples used in the calculations, the variance of the sample mean would be biased if (7) was used. Based on the results described in the Appendix, the variance of the sample mean can be calculated using (A8) with the substitution $K = N - L$. This estimate is unbiased for white noise disturbances. For colored noise disturbances simulations show that the bias in the variance estimate is present, but the compensation still provides acceptable results.

IV. Simulation Results

In this section, the operation and performance of the proposed algorithm are illustrated through simulation examples.

Error Surface: Fig. 3 illustrates the error surface (2) as a function of the frequency estimator. In the example a multisine was used with 40 harmonics, with uniform amplitudes. The fundamental and the sampling frequencies were $f_0 = 100$ Hz and $f_s = 10$ kHz. The LS solution was calculated for different values of the frequency estimator, as shown on the plot. The inset illustrates that the shape of the error surface is close to a parabola in case the estimate is close to the true value. The figure also illustrates the necessity of a good starting value; otherwise, the iteration may end in a local minimum.

The following simulations illustrate the behavior of the proposed algorithm and compare it to the matrix-based method [1]. In all the simulations, the iteration was finished when the relative residual error was below $1 \cdot 10^6$ (see the exit criterion in step N5 for the resonator-based case). The number of harmonics was close to the maximum ($f_s/2f_0$).

Example 1: In this simulation, the frequency estimators and the residual errors of the two algorithms are compared. The fundamental frequency of the input signal $f_0 = 105$ Hz, the sampling frequency $f_s = 10$ kHz, and the number of harmonics $M = 45$. All of the spectral components have equal amplitudes ($|A_m| = 1$, random phase) and the variance of the additive noise is $\sigma^2 = 10^{-2}$. The number of points in the record varied from $N = 110$ (1.15 periods) to $N = 1000$ (10.5 periods). Table I shows the estimators of the fundamental frequency and the residual errors for the matrix-based algorithm [1] and for the proposed resonator-based method. It is clearly visible that the two algorithms gave very similar results. The difference is due to the fact that the resonator-based method uses the sample mean values as amplitude estimators, instead of the true LS solution.

Example 2: The convergence rates of the two algorithms are compared in Fig. 4, where the frequency error is shown as a function of the iteration steps. The test signal was similar to that of Example 1, but now it contained 10 000 samples. The initial frequency estimator was 105.1 Hz for the matrix-based method

TABLE I
FREQUENCY ESTIMATES AND RESIDUAL ERRORS OF THE TWO NLS ALGORITHMS

	Matrix-based [1]		Resonator-based	
N	$\hat{f}_0$	E^2	$\hat{f}_0$	E^2
110	104.984	571	104.986	574
200	104.991	1150	104.993	1153
500	104.998	2872	104.998	2876
1000	105.001	6021	105.001	6028

and 105.1 Hz with two additional points at 105.1 ± 0.01 Hz for the resonator-based algorithm. The behaviors of the algorithms again were quite similar.

Example 3: The computational complexity of the two algorithms is compared in Table II, where the numbers of floating-point operations (flops in Matlab) are shown for one iteration step, using different input data. The results illustrate the complexity of the algorithms: the matrix-based method requires $O(NM^2)$ operations while the resonator-based method only $O(NM)$. The evaluation times are also shown (Matlab, Pentium III with 256 Mbyte memory). It is clearly visible that the built-in matrix calculations provide faster execution for the matrix-based algorithm for smaller data sizes, although the number of calculations is higher.

Notes

- The results shown in Table II apply to one iteration step. The necessary number of iterations usually varies between 3–15, depending on the input signal and the initial frequency estimations. For the same initial conditions, the numbers of iterations of the algorithms are usually close to each other.
- The resonator-based algorithm does not require the implementation of any matrix-based calculations. This makes it extremely easy-to-implement on a low-level (DSP, or programmable logic arrays).
- If the number of harmonics is known *a priori* and it is much lower than the possible number of harmonics, then the matrix-based method can spare calculations (M is the number of the harmonics actually present). In the case of the resonator-based method, it is also possible, but from a numerical point of view it is more advisable, to use almost equally distributed resonators, i.e., to use all the possible harmonics ($M \approx f_s/2f_0$).

Example 4: In these simulations, the variance estimators are illustrated for white and colored disturbances. For white additive noise with variance $\sigma^2 = 10^{-2}$, Fig. 5 shows the variance estimators of the sample mean calculated by the resonator-based algorithm, using the two different calculation methods (7) and (A8), for different numbers of periods present in the record. The results gained from the block-wise and the sample-wise calculation methods are very similar and they are close to the true value, too.

When the noise is colored, the sample-wise estimator is biased, as illustrated in Fig. 6. In case of multiple periods, the estimates (both the block-wise and the sample-wise) are close to the true value, while for short data records (1.2 periods in the example), the sample-wise estimator has a large bias. However, the estimate still provides information on the shape of the noise.

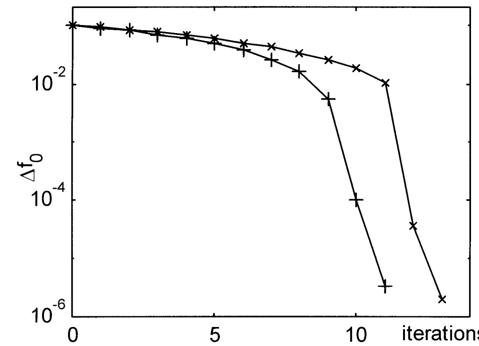

Fig. 4. Convergence of frequency estimator of two NLS algorithms. $+$: resonator-based; $\times$: matrix-based method.

TABLE II
COMPUTATIONAL LOAD PER ITERATION OF THE TWO NLS ALGORITHMS

		Matrix-based [1]		Resonator-based	
N	M	flops	Time	flops	Time
200	50	$5.0{\cdot}10^7$	0.6s	$4.4{\cdot}10^6$	1.4s
1000	50	$2.5{\cdot}10^8$	4.5s	$2.2{\cdot}10^7$	5.3s
1000	100	$9.7{\cdot}10^8$	17s	$4.4{\cdot}10^7$	8.3s
1000	400	$1.7{\cdot}10^{10}$	4.7min	$1.7{\cdot}10^8$	1.0min
5000	400	$8.1{\cdot}10^{10}$	26.7min	$8.7{\cdot}10^8$	2.7min
5000	2000	out of memory		$4.5{\cdot}10^9$	26min

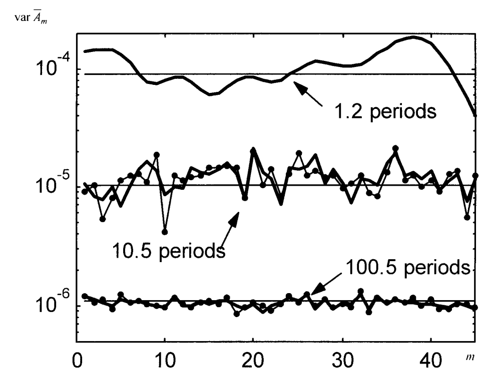

Fig. 5. Variance of the sample mean, calculated by the sample-wise (thick lines) and the block-wise (thin lines with dots) methods. Solid thin lines show the theoretical values (white noise).

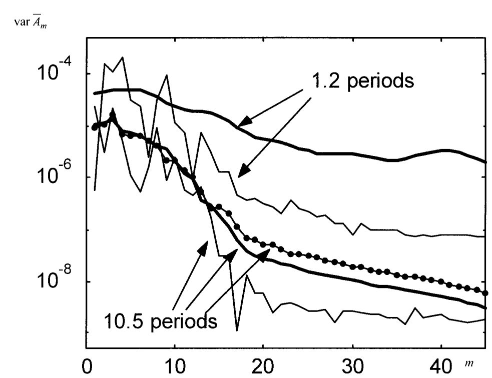

Fig. 6. Biased variance of the sample mean, calculated by the sample-wise (thick lines) and the block-wise (thin lines with dots) methods. Solid thin lines show the shape of the colored noise.

Note that the variance estimators together with the sample mean can be used to determine the frequency components present in the signal, as described in [4].

V. Conclusion

A new solution was proposed to solve the nonlinear least squares problem for periodic signal estimation. The proposed algorithm uses recursive model-based computation techniques, which enable the reduction of both the computational cost and the memory requirements of the algorithm. The structure of the algorithm makes it especially suitable for low-level (hardware or DSP) implementation.

The proposed new calculation method has the following properties compared to the conventional (matrix-based) calculation:

- The new algorithm requires only $O(MN)$ operations and $O(N)$ storage space, in contrast with the $O(NM^2)$ operations and $O(NM)$ memory requirement of the conventional method, where N is the length of the data record and M is the number of frequency lines.
- For long data records the sample mean and variance estimates are the same as in the conventional approach, but no segmentation, synchronization, and re-estimation are required.
- For short data records, when the sample variance estimation is not possible using the conventional block-approach, the new algorithm still gives good estimates for the sample variance. For white noise, the estimate is unbiased. In case of colored noise the estimator has bias, but follows the noise shape, according to simulations.

Appendix
Variance of the Sample Mean

For sake of simplicity, the calculations are made for the dc component A_0, but for all the spectral components A_m, the calculation can be similarly carried out by inserting the appropriate phase components.

Let's denote the estimate of spectral component at time instant $k+L-1$ by

$$A_0^{[k]} = A_0(k+L-1) = \frac{1}{L}\sum_{i=k}^{k+L-1} s(i) \tag{A1}$$

where $s(i) = \hat{s}(i) + e(i)$ is the noisy observed input. The noise $e(i)$ is white with zero mean and variance σ^2. If $E_0^{[k]} = 1/L\sum_{i=k}^{k+L-1} e(i)$, then the variance and cross-correlation terms of the noise spectrum are the following:

$$E\left\{\left(E_0^{[k]}\right)^2\right\} = E\left\{\left(\frac{1}{L}\sum_{i=k}^{k+L-1} e(i)\right)^2\right\} = \frac{L\sigma^2}{L^2} \tag{A2}$$

$$\begin{aligned} E\left\{\left(E_0^{[k_1]}\right)\left(E_0^{[k_2]}\right)\right\} =& E\left\{\left(\frac{1}{L}\sum_{i=k_1}^{k_1+L-1} e(i)\right)\right. \\ &\left.\cdot\left(\frac{1}{L}\sum_{i=k_2}^{k_2+L-1} e(i)\right)\right\} \\ =& \begin{cases} \frac{(L-|k_1-k_2|)\sigma^2}{L^2} & \text{if } |k_1-k_2| < L \\ 0 & \text{if } |k_1-k_2| \ge L \end{cases} \end{aligned} \tag{A3}$$

where $E\{\cdot\}$ denotes the expected value operator. The sample variance of A_0 can be computed as follows.

$$\begin{aligned} \hat{\sigma}^2(A_0) =& \frac{1}{K-1}\sum_{k=1}^{K}\left|A_0^{[k]} - \frac{1}{K}\sum_{k_1=1}^{K} A_0^{[k_1]}\right|^2 \\ =& \frac{1}{K-1}\sum_{k=1}^{K}\left|E_0^{[k]} - \frac{1}{K}\sum_{k_1=1}^{K} E_0^{[k_1]}\right|^2. \end{aligned} \tag{A4}$$

Using (A2) and (A3), the expected value of $\hat{\sigma}^2(A_0)$ can be calculated [see (A5) at the bottom of the page], where

$$f_k = \begin{cases} k & \text{if } 1 \le k \le \min(L,K) \\ \min(L,K) & \text{if } \min(L,K) < k \le \max(L,K) \\ L+K-k & \text{if } \max(L,K) < k \le K+L-1 \end{cases} \tag{A6}$$

The variance of the sample mean is

$$\begin{aligned} \mathrm{var}\bar{A}_0 =& E\left\{\left(\bar{A}_0 - E\left\{\bar{A}_0\right\}\right)^2\right\} = E\left\{\left|\frac{1}{K}\sum_{k=1}^{K} E_0^{[k]}\right|^2\right\} \\ =& \frac{\sigma^2}{L^2K^2}\sum_{k=1}^{K+L-1} f_k^2. \end{aligned} \tag{A7}$$

The estimate of the variance of the sample mean can be expressed from (A5) and (A7) [see (A8) at the top of the next page]. (A8) will be an unbiased estimator in case of white noise disturbances.

$$\begin{aligned} E\left\{\hat{\sigma}^2(A_0)\right\} =& \frac{\sigma^2}{K-1}\cdot\left(\frac{KL}{L^2} + \frac{1}{K}E\left\{\left(\sum_{k=1}^{K} E_0^{[k]}\right)^2\right\} - \frac{4}{KL^2}\sum_{i=1}^{\min(K,L)}(K-i)(L-i) - \frac{2L}{L^2}\right) \\ =& \frac{\sigma^2}{L^2(K-1)}\left(KL - 2L + \frac{1}{K}\sum_{k=1}^{K+L-1} f_k^2 - \frac{4}{K}\sum_{i=1}^{\min(K,L)}(K-i)(L-i)\right) \end{aligned} \tag{A5}$$

$$\hat{\sigma}^2\left(\bar{A}_0\right)=\hat{\sigma}^2\left(A_0\right)\frac{(K-1)}{K^2}\sum_{k=1}^{K+L-1}f_k^2\frac{1}{KL-2L+\frac{1}{K}\sum\limits_{k=1}^{K+L-1}f_k^2-\frac{4}{K}\sum\limits_{i=1}^{\min(K,L)}(K-i)(L-i)} \tag{A8}$$

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