



Error Analysis in Determining Parameters of Overlapping Peaks Using Separation of Complex Spectra into Individual Components Case Study: Triplets

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Abstract: Based on the concept of Big Data Modeling, the errors in determining peak parameters of noisy Gaussian triplets using nonlinear least squares curve fitting have been evaluated. Calculations were performed using Gauss-Newton (with Levenberg-Marquardt modifications) and genetic algorithms. The probability that the relative error in estimating each model parameter is not greater than a priori given limit for a given fitting error has been calculated. It was shown that using the derivative mode for curve fitting has no advantage over the normal mode. It was demonstrated that the mean errors for the genetic algorithm are significantly greater than for the Gauss-Newton algorithm. It was found that the mean probability for triplets is higher than that for quartets. Obtained results showed that small fitting error does not guarantee that a fitting algorithm does converge to the correct peak parameters.

Keywords: spectrochemistry, overlapping peaks, curve fitting, Gauss-Newton and genetic algorithms, errors of peak parameters

I. Introduction

Mathematical separation of overlapping analytical signals (peaks) is one of the widely used pre-processing methods in spectroscopy and chromatography (see references in [1]). Numerous computer-based algorithms have been developed to solve the separation problem (e.g., derivative spectroscopy and other peak sharpening methods). However, the most mathematically rigorous curve-fitting procedures for separation of badly resolved peaks are based on the fitting a priori model to the experimental data using the Gauss-Newton regression algorithm with Levenberg-Marquardt modifications (in what follows the Gauss-Newton algorithm) and genetic algorithm [2]. Curve-fitting model parameters are served as raw data for the qualitative and quantitative analysis. It is well known that the process of determining parameters of overlapping peaks in the case of uncertainty in the measured data is represented mathematically as an inverse ill-posed problem [3]. This problem can be solved only by using *a priori* information about the exact solution. Therefore, generally speaking, it was pointed out that one can only evaluate the probability (Ψ_{P_i}) that the relative error in estimating parameter P_i of i^{th} peak is not greater than a given value for a given fitting error [4].

The previous paper [4] dedicated to the error analysis in determining parameters of unresolved peaks was based on the concept of Big Data Modeling [5]. We studied 771,750 Gaussian quartets which set of the parameters covered most common values. Although it is impossible to mimic all practical situations (a population) encountered in spectra, general qualitative and quantitative patterns have been obtained. It was shown that small fitting error does not guarantee that a fitting algorithm does converge to the correct peak parameters. The relationships between the mean probability over all quartet parameters and the parameters of the Gauss-Newton algorithm have been established. It was found that the probability Ψ_{P_i} strongly depends on the sample of quartets taken from the entire population.

It is impossible to increase essentially the size of the quartet population since the decomposition process is a very time consuming. However, the set of possible values of peak parameters may be significantly increased using triplets despite that their number decreases. "Small" size of a set of triplets allows studying the genetic algorithm which is significantly time consuming as compared to the Gauss-Newton method. Also it is interesting to compare results obtained for quartets and triplets.

In this paper we present an analysis of the errors in determining peak parameters of overlapping peaks using the least squares decomposition of complex spectra into individual components. Decomposition was carried out via the Gauss-Newton and the genetic algorithm. The spectra were simulated by the 254,016 combinations of three Gaussian peaks which parameters are varying in a very large range.

In what follows, for the sake of simplicity, term "line" is used instead of terms "peak, line and band". The standard algebraic notations are used throughout the article. All calculations were performed and the plots were built using the MATLAB software.

II. Computer Modeling

Multiline spectra were simulated by Gaussian triplets:

$$Q(x) = \sum_{i=1}^3 F(x, x_{0i}, R_i, r_i), \quad (1)$$

where $F(x, x_{0i}, R_i, r_i) = R_i \exp\{-(x - x_{0i})/r_i\}^2\}$ is the i^{th} line; $x = 2\sqrt{\ln 2}j, j = [-7:0.02:7]$, x_{0i}, R_i and r_i are the position of the maximum, the relative intensity and the relative width of the i^{th} line, respectively. Parameter values of triplets are given in Table 1 (total number of combinations $N_{\text{total}} = 254,016$). High and low resolution spectra of triplets and their first-order derivatives are shown in Fig. 1.

Table 1. Parameter values

Parameter	x_{02}	$-x_{01}, x_{03}$	R_2	R_1, R_3	r_2	r_1, r_3
Values	0	0.3:0.1:1	1	0.1, 0.2, 1/3, 0.5, 1, 2, 3, 5, 10	1	0.2, 1/3, 0.5, 1, 2, 3, 5

Curve fitting (non-linear regression) to three Gaussian lines was performed using Gauss-Newton (MATLAB function *nlinfit*) and genetic (MATLAB function *ga*) algorithm. The first algorithm was also applied to the first-order derivative of the triplets (the derivative mode).

For the Gauss-Newton algorithm the initial values of parameters (P_i^{init}) except $P_{x_{02}}^{\text{init}}$, were equal to

$$P_i^{\text{init}} = LB + (UB - LB)\eta, \quad (2)$$

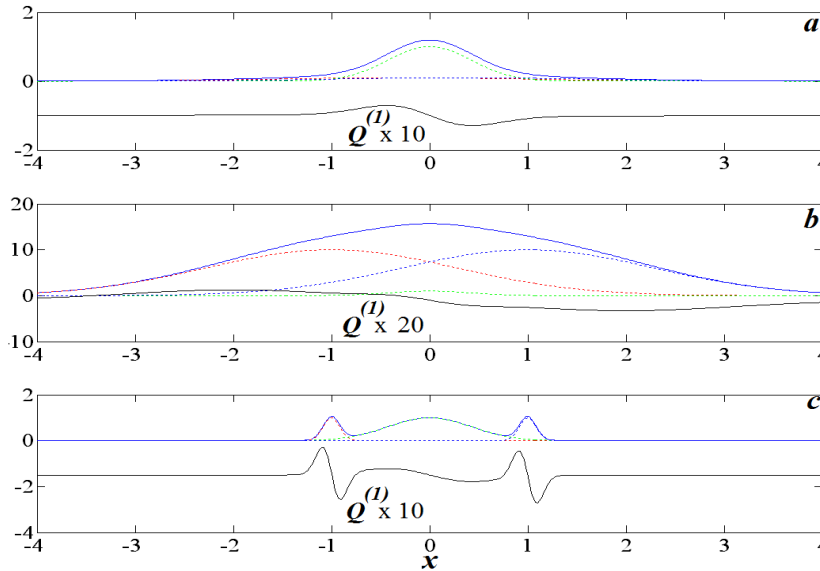
where $LB = P_i^{\text{true}} lLim$ and $UB = P_i^{\text{true}} uLim$ are the low and the upper bounds, respectively; P_i^{true} is a true parameter value; $lLim$ and $uLim$ are $1 \mp lim$, respectively; $lim=0.2$ and 0.5 ; η is a random variable uniformly distributed in the range 0-1.

Since the true value of x_{02} is zero, then its initial value

$$P_{x_{02}}^{\text{init}} = -lim + 2lim \eta \quad (3)$$

For genetic algorithm the range of parameter values: $P_i = [LB, UB]$ except $P_{x_{02}} = [-lim, lim]$.

Figure 1. Spectral triplets and their first-order derivatives



$[x_{01}, R_1, r_1, x_{03}, R_3, r_3] = [-0.3, 0.1, 3, 0.3, 0.1, 3]$ (a), $[-1, 10, 3, 1, 10, 3]$ (b) and $[-1, 1, 0.2, 1, 1, 0.2]$ (c).

Random noise with zero mean and standard deviation $\sigma = 0.01$ was added to the each triplet (1). $\sigma = 0.002$ for low noise triplets. At the next step triplet parameters were estimated. For randomization these two procedures were repeated 20 times. We studied two cases:

1. Unconstrained non-linear regression (UR) when whole curve-fitting data was considered valid.
2. Constrained regression (CR). In the case of the rank deficient program warnings of the Gauss-Newton algorithm and when the maximum number of generations of genetic algorithm exceeded, the obtained data was rejected. In both cases the following soft constraints were applied:

$$x_{01} < 0, x_{03} > 0, R > 0, r > 0 \quad (4)$$

The relative error (%) in estimating parameter P_i is equal to

$$\xi_{P_i} = 100(\bar{P}_i^{\text{estim}} - P_i^{\text{true}})/P_i^{\text{true}}, \quad (5)$$

where $\bar{P}_i^{\text{estim}}$ is the mean value of the P_i^{estim} -values.

The fitting error:

$$\xi_{\text{fit}} = \sqrt{\sum_{j=1}^{701} (Q(x_j) - \hat{Q}(x_j))^2 / 701}, \quad (6)$$

where $\hat{Q}(x_j)$ is obtained from Eq. 1 by substituting $\bar{P}_i^{\text{estim}}$.

The indicator for good model fit was

$$\xi_{fit} \leq K_{noise} \sigma, \quad (7)$$

where K_{noise} is the noise multiplier. The number of the good-fitting models $N_{gf} < N_{total}$. From these models only those triplets for which

$$\xi_{P_i} \leq K_\xi, \quad (8)$$

have been chosen. $K_\xi = [20, 10, 5, 1]$ for all P_i , except P_{x02} for which $K_\xi = [0.05, 0.025, 0.01, 0.002]$.

Number of selected triplets depends on the coefficients $K(N(K_{noise}, K_\xi))$. The relative value (%):

$$\Psi_{gf} = 100N(K_{noise}, K_\xi)/N_{gf} \quad (9)$$

has been calculated. It was shown in [4] that Ψ_{gf} may be considered as the probability that the relative error in estimating parameter P_i is not greater than K_ξ for a given ξ_{fit} over good fit. Also we found that the mean probability $\bar{\Psi}_{gf}$ weakly depends on the sample taken from the entire population of Gaussian quartets.

III. Results and Discussion

Typical histograms of the ξ_{P_i} distributions for $K_{noise}=3$ are given in Figs. 2-6. These plots are usually asymmetric unimodal, however for $lim=0.5$ two modes appear for R_2 and r_2 in the case of the Gauss-Newton algorithm. For genetic algorithm the histogram shapes are differ from the corresponding histograms of the Gauss-Newton algorithm. This result is due to different use of initial parameters for both algorithms.

It is seen from the histograms that the number of the good-fitting models (N_{gf}) significantly decreases for $lim=0.5$ as compared to $lim=0.2$.

Table 2 represents the statistical parameters (mean, variance and skewness) of the error distributions. It is seen from this table that for experiments based on the unconstrained regression the absolute value of mean errors $|\bar{\xi}_{P_i}|$ increase if the range bounds of initial guesses increase (lim increases from 0.2 to 0.5).

For experiments based on constrained regression (Eq. 4), the size of the sets meet the given constraints, decreases. For these sets $|\bar{\xi}_{P_i}|$ decreases as expected. The exceptions are $|\bar{\xi}_{R_3}|$ and $|\bar{\xi}_{r_3}|$ for $lim=0.2$ and 0.5, respectively. For the Gauss-Newton algorithm the values of $|\bar{\xi}_{P_i}|$ in the derivative mode increase as compared to the normal mode.

Figure 2. Histograms of the error distribution for Gauss-Newton algorithm ($lim = 0.2$)

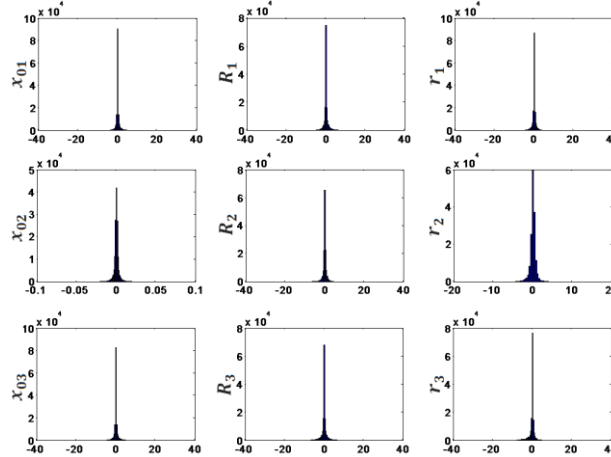


Figure 3. Histograms of the error distribution for Gauss-Newton algorithm ($lim = 0.5$)

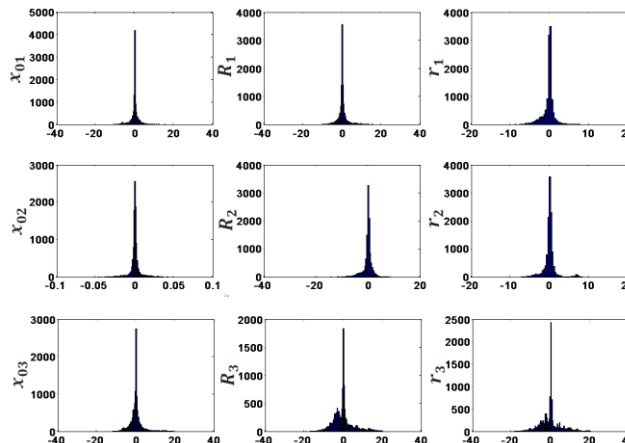
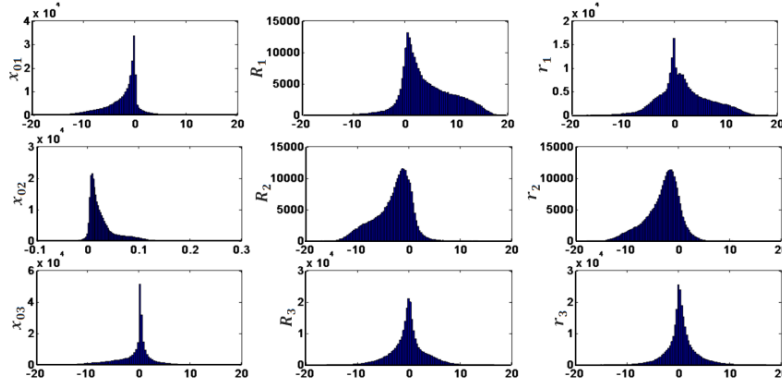
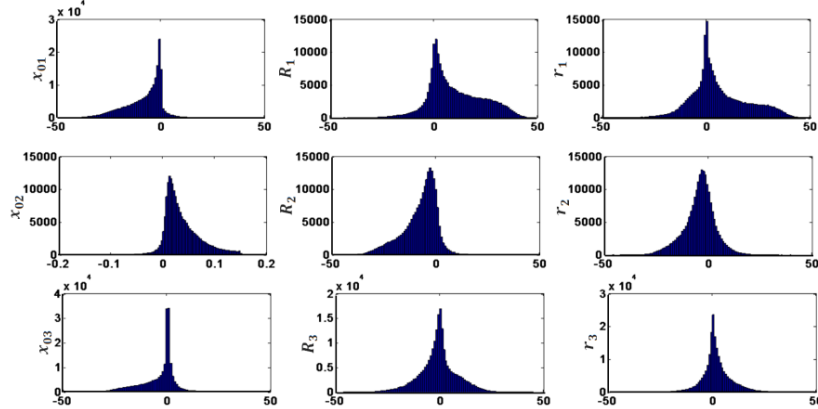


Figure 4. Histograms of error distribution for genetic algorithm ($lim = 0.2$)Figure 5. Histograms of the error distribution for genetic algorithm ($lim = 0.5$)

The mean errors for the genetic algorithm are significantly greater than for the Gauss-Newton method (Table 2). As expected, the mean errors of triplets are less than corresponding errors for quartets [4].

No dependence of skewness upon the errors of modeling parameters has been found.

Fig. 6 shows that in the most cases the correlation between errors is low.

The relative error probability is a very complex function $\Psi_{gf}(P_i, lim, K_{noise}, K_{\xi})$. Tables 3 and 4 represent some numerical values of this function for Gauss-Newton and genetic algorithms. From these tables the following conclusions can be drawn:

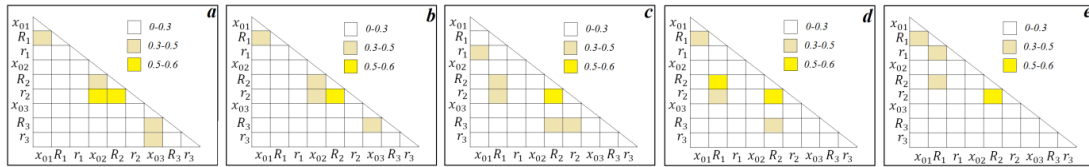
1. For both algorithms probability Ψ_{gf} increases while increasing K_{ξ} . The dependence $\Psi_{gf}(K_{noise})$ is

Table 2. Statistical parameters of the error distributions ($K_{noise} = 3$)

lim	Regression	Parameters of triplets									
		x_{01}	R_1	r_1	x_{02}	R_2	r_2	x_{03}	R_3	r_3	
Gauss-Newton algorithm. Normal mode											
0.2	UR	- 0.074± 0.016	-0.24± 0.017	-0.73± 0.017	0	-0.39± 0.015	-0.23± 0.009	- 0.089± 0.016	-0.25± 0.017	-0.75± 0.017	
		0.23	-0.43	-2.9	-0.36	-1.0	-2.4	0.079	-0.43	-2.8	
	CR	- 0.061± 0.014	0	-0.33± 0.010	0	-0.38± 0.015	-0.26± 0.007	- 0.059± 0.016	- 0.072± 0.017	-0.80± 0.017	
		0.071	1.0	-1.8	-0.69	-1.1	-1.1	0.65	0.75	-2.4	
	0.5	UR	-1.05± 0.13	-0.24± 0.11	-1.61± 0.11	0	-1.05± 0.082	0.38± 0.079	-1.14± 0.13	- 0.041± 0.11	-1.63± 0.12
			-0.97	-0.26	-1.7	-0.21	-1.21	0.15	-1.1	0	-1.7
UR		-0.11±	-0.14±	-0.26±	0	-0.11±	-	-0.18±	-0.10±	-0.27±	

	<i>low noise</i>	0.063	0.043	0.044		0.028	0.067± 0.015	0.058	0.050	0.045
		2.0	0	-6.9	-0.26	3.5	-0.61	1.7	1.9	-7.1
	CR	0	0.11± 0.073	-0.53± 0.051	0	-0.76± 0.066	-0.19± 0.042	0	-0.33± 0.11	-0.43± 0.11
		0.52	0.89	-0.94	-0.30	-1.7	0.38	0.84	0.26	0
Gauss-Newton algorithm. Derivative mode										
0.5	UR	-1.03± 0.23	-1.94± 0.27	0.72± 0.24	0	-4.16± 0.29	3.53± 0.25	-0.97± 0.23	-1.67± 0.26	0.52± 0.23
		0.93	-1.7	1.0	-0.22	-1.3	1.31	-0.92	-1.7	0.82
		0	-1.88± ±0.12	0.71± 0.18	0	-4.77± 0.32	2.31± 0.16	-1.14± 0.19	-1.33± 0.30	1.30± 0.33
	CR	0.69	-2.0	1.9	-0.73	-1.2	1.3	-0.51	-0.77	0.85
	Genetic algorithm. Normal mode									
0.2	CR	-2.67± 0.025	3.98± 0.037	1.58± 0.023	0.025± 0.0002	-3.34± 0.030	-3.35± 0.030	-1.01± 0.016	-0.42± 0.013	0.17± 0.011
		-1.5	1.4	1.5	1.5	-1.3	-1.3	-1.8	-0.82	0.56
		-8.63± 0.086	9.6± 0.10	5.46± 0.076	0	-8.25± 0.081	-4.77± 0.054	-4.37± 0.055	-1.43± 0.041	1.43± 0.034
0.5	CR	-1.4	1.4	1.6	1.3	-1.3	-1.5	-1.7	-0.96	1.3

Figure 6. Linear correlation coefficients between errors

Genetic algorithm: ($lim=0.2$ (a), 0.5 (b)). Newton-Gauss algorithm: normal mode ($lim=0.2$ (c), 0.5 (d)), derivative mode ($lim=0.5$ (e))

decreasing for the Gauss-Newton algorithm; however, for genetic algorithm it is increasing in many cases (red numbers in Table 4). Contrary to the Gauss-Newton algorithm it is rapidly approaching saturation at small values of $K_{noise} = 3 \div 5$.

2. The mean probability $\bar{\Psi}_{gf}$ for $lim=0.2$ is higher than that for $lim=0.5$.

3. Constrained regression increases the values of $\bar{\Psi}_{gf}$.

4. The mean probability $\bar{\Psi}_{gf}$ decreases in the derivative mode as compared with the normal mode. This result contradicts the conclusion of [6]. In this article it was pointed out that a chance of finding accurate values of line parameters increases with increasing resolution in the first-order derivative. However, the noise enhancement due to the differentiation decreases the probability Ψ_{gf} .

5. There is no general relationship between whose probabilities which satisfied the condition $\Psi_{gf} < 0.95 * \bar{\Psi}_{gf}$ and triplet parameters. However, for constrained regression when $lim=0.5$ this condition is true for R_2 and r_2 in both modes. Only one exception exists. So, the intensity and the width of the middle triplet line are the most error-sensitive triplet parameters in decomposition process.

6. The mean probability $\bar{\Psi}_{gf}$ [4] for quartets is significantly less than that for triplets (Table 5).

We tried to find correlation between probabilities Ψ_{gf} and multivariate selectivity in terms of the net analyte signal [7]. Unfortunately, no correlation has been found.

Like we mentioned in the previous article [4], obtained results show that a small fitting error does not guarantee that a fitting algorithm does converge to the correct line parameters. E.g., for constrained regression, using Newton-Gauss algorithm in the normal mode for $lim=0.5$, the minimal probability that the absolute value of the relative errors in determining parameters is less than 5%, $\Psi_{gf}^{min}=61.1\%$. For $lim=0.2$ $\Psi_{gf}^{min}=87.2\%$. If $K_{noise} = 1$ then $\Psi_{gf}^{min}=65.6\%$ and 30.7 for $lim=0.2$ and 0.5 , respectively. Moreover, in the case of small fitting errors, the relative number of the good model fits decreases significantly (Table 6).

In conclusion, probability Ψ_{gf} increases when the initial guesses are close to the exact values of the parameters and noise decreases. In analytical practice the probability Ψ_{gf} can be increased by averaging of parameters obtained from multiple repetitions of the same experiment.

Table 3. Relative error probability (Ψ_{gf}) for Gauss-Newton algorithm

lim	Regression	K_{ξ}	Mode	Parameters									
				x_{01}	R_1	r_1	x_{02}	R_2	r_2	x_{03}	R_3	r_3	mean
0.2	UR	20	normal	95.4	94.5	96.3	95.4	94.4	96.2	98.5	98.8	100.0	96.6
				91.6	90.5	93.3	91.6	90.4	93.3	94.0	94.8	99.4	93.0
		10		92.1	90.7	92.8	92.0	90.6	92.9	95.1	95.9	99.1	93.5
				87.1	85.2	88.8	87.1	85.2	88.9	88.3	89.6	96.4	88.5
		5		87.3	85.7	89.3	87.3	85.5	89.3	88.1	91.5	97.2	89.0
				81.4	78.9	84.4	81.4	78.8	84.4	79.8	83.5	91.4	82.7
		1		72.0	67.8	74.2	71.9	67.7	74.1	62.6	73.5	80.3	71.6
				65.5	61.1	68.8	65.5	61.0	68.7	55.3	65.1	71.0	64.7
	CR	20		97.9	97.4	99.8	97.0	95.8	96.4	98.7	98.9	100.0	98.0
				96.5	95.6	99.4	95.4	93.0	90.8	96.1	96.1	99.8	95.9
		10		95.5	94.9	98.9	94.0	92.5	93.7	95.8	95.9	99.8	95.7
				93.3	92.1	97.7	91.6	87.9	86.1	91.6	91.5	98.5	92.3
		5		91.7	90.7	96.2	89.6	87.2	88.8	89.6	91.9	98.5	91.6
				88.7	87.1	94.1	86.4	80.7	79.6	84.4	86.6	92.2	87.0
		1		77.1	72.3	79.9	73.3	67.1	70.9	65.6	75.4	85.2	74.1
				73.6	68.0	76.9	69.2	59.5	61.3	61.5	70.3	80.2	68.9
0.5	UR	20	normal	71.8	74.2	77.1	71.6	73.5	76.9	92.4	98.0	99.7	81.7
				56.7	59.6	64.5	56.8	59.7	64.6	67.0	86.3	91.8	67.5
			derivative	74.3	64.8	65.3	73.9	64.9	65.0	92.4	97.1	100.0	77.5
				56.9	52.8	56.2	57.1	53.0	55.9	64.9	81.4	90.4	63.2
		10	normal	61.1	66.0	68.5	60.6	65.3	68.0	75.6	91.5	92.5	72.1
				44.2	49.6	54.5	44.3	49.5	54.7	46.5	69.5	71.3	53.8
			derivative	64.7	56.1	54.9	64.4	56.5	54.9	76.2	87.6	90.5	67.3
				43.8	42.8	45.0	44.6	42.8	44.9	44.5	58.6	68.5	48.4
		5	normal	49.7	56.2	59.7	48.8	55.6	59.5	53.1	78.6	75.6	59.6
				31.6	38.9	44.5	31.6	38.8	44.6	28.5	50.5	49.3	39.8
			derivative	51.8	48.6	49.1	52.1	49.1	49.8	46.2	60.9	64.1	52.4
				30.6	33.4	36.5	31.6	33.4	36.6	23.9	34.9	43.9	33.9
		1	normal	29.9	35.4	40.0	29.2	34.3	40.0	29.1	42.1	39.0	35.4
				16.5	19.9	23.8	16.3	19.5	23.9	13.1	21.4	19.9	19.4
			derivatives	27.9	32.3	35.5	29.5	33.2	36.5	16.9	9.1	8.6	25.5
				14.1	17.8	19.8	14.3	18.3	19.9	8.1	5.6	7.3	13.9
	CR	20	normal	95.9	96.6	97.2	94.8	90.5	92.2	96.4	98.4	99.9	95.8
				91.3	90.4	88.1	89.4	70.7	64.8	83.5	92.8	98.5	85.6
			derivative	97.4	96.1	91.5	89.1	75.5	68.5	96.0	97.8	99.9	90.2
				90.5	88.0	83.4	78.2	52.7	49.0	81.8	91.6	97.9	79.3
		10	normal	90.3	91.2	95.4	87.7	80.3	80.0	89.1	94.8	99.0	89.8
				83.0	81.6	83.6	77.8	53.7	48.2	71.0	83.1	92.7	75.0
			derivative	93.6	87.5	81.2	80.4	56.8	47.5	86.0	89.2	98.3	80.1
				81.6	75.3	72.3	63.9	35.8	31.0	65.8	76.7	89.8	65.8
		5	normal	80.7	82.5	90.5	77.3	63.5	61.1	77.9	87.8	92.7	79.3
				69.4	70.1	75.0	61.7	35.2	31.2	57.8	70.7	80.5	61.3
			derivative	83.9	78.7	75.8	65.5	40.3	34.6	62.7	65.3	92.3	66.6
				66.7	62.3	62.7	45.5	21.9	18.8	45.3	51.2	75.6	50.0
		1	normal	55.4	56.4	66.2	44.3	30.7	32.5	52.6	61.5	72.8	52.5
				43.9	42.6	49.3	29.1	13.4	13.4	36.0	44.1	53.6	36.1
			derivative	52.7	54.3	50.6	30.8	19.3	17.9	27.4	3.4	9.7	29.6
				37.4	36.9	36.8	16.2	7.0	6.8	19.2	4.5	10.2	19.4

$K_{noise} = 3$ and 10 for upper and lower rows, respectively. Values $\Psi_{gf} < 0.95 * \bar{\Psi}_{gf}$ are given in bold italic.

Table 4. Relative error probability (Ψ_{gf}) for genetic algorithm

lim	K_{ξ}	Parameters									
		x_{01}	R_1	r_1	x_{02}	R_2	r_2	x_{03}	R_3	r_3	mean
0.2	20	100.0	100.0	100.0	100.0	90.8	100.0	100.0	100.0	100.0	99.0
		100.0	100.0	100.0	100.0	84.3	100.0	100.0	100.0	100.0	98.3
		100.0	100.0	100.0	100.0	83.9	100.0	100.0	100.0	100.0	98.2
	10	94.8	80.6	90.3	74.9	95.2	96.9	97.1	99.1	99.3	92.0
		95.7	84.4	92.1	64.5	94.7	95.7	97.5	99.1	99.4	91.4
		95.8	84.5	92.2	64.0	94.6	95.6	97.5	99.1	99.4	91.4
	5	75.9	53.8	65.7	37.7	76.6	81.1	82.9	86.5	90.4	72.3

0.5	1	79.4	60.5	70.2	31.1	72.8	74.9	84.6	86.8	90.8	72.3
		79.5	60.9	70.4	30.8	72.7	74.7	84.6	86.9	90.8	72.4
		31.5	18.6	22.7	4.0	25.2	22.0	49.0	37.5	45.3	28.4
		36.4	21.4	24.5	3.4	23.2	19.4	50.5	39.3	45.6	29.3
		36.6	21.6	24.5	3.4	23.2	19.3	50.6	39.4	45.6	29.3
	20	82.9	57.4	72.9	86.6	98.0	99.9	89.3	97.2	86.6	86.9
		85.7	71.2	78.6	75.1	91.8	98.0	92.0	96.1	97.7	87.3
		87.2	74.9	80.8	67.3	89.7	96.3	92.4	95.8	97.5	86.9
	10	56.2	36.6	51.3	62.8	82.4	95.6	72.4	75.3	84.4	68.5
		61.8	49.2	58.3	48.6	71.7	83.6	76.1	75.6	84.3	67.7
		65.0	53.3	60.5	42.6	67.5	78.3	76.7	75.8	84.3	67.1
	5	38.1	24.9	31.7	23.3	56.1	73.4	60.2	48.5	63.3	46.6
		42.6	33.8	38.8	17.5	46.4	55.8	61.6	51.8	64.1	45.8
		45.9	36.6	40.8	15.4	43.0	50.7	61.9	52.9	64.2	45.7
	1	13.2	8.4	10.9	3.1	13.5	17.4	32.5	14.5	21.8	15.0
		15.2	10.6	13.5	2.5	11.0	12.3	32.7	16.4	23.2	15.3
		16.6	11.2	13.8	2.3	10.2	11.1	32.7	16.9	23.0	15.3

$K_{noise} = 1, 2$ and 3 from upper to lower rows, respectively. Values $\psi_{gf} < 0.95 * \bar{\psi}_{gf}$ are given in bold italic

Table 5. Comparison of the mean relative error probabilities for triplets and quartets decomposed by Gauss-Newton algorithm

K_{ξ}	20	10	5	1
Triplets	95.8	89.8	79.3	52.5
	85.6	75.0	61.3	36.1
Quartets	94.7	85.6	68.7	32.9
	81.7	65.0	45.8	18.3

$K_{noise} = 3$ and 10 for upper and lower rows, respectively. $lim = 0.5$.

Table 6. Relative number of the good model fits ($N_{gf}/N_{total}, \%$)

K_{noise}	Regression	lim	
		0.2	0.5
3	UR	70.8	6.2
	CR	66.3	5.4
10	UR	85.8	24.8
	CR	79.0	8.8

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