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LIMITS AND ACCURACY IN MEASUREMENTS

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1 Introduction

The word **ACCURACY** (from Lat. accuratus – made with taking care of) has several definitions:
- the freedom from errors;
- property of a human statement to be adequate to truth;
- degree of conformity of a measurement to a true value, i.e to a standard or to a model;
which are reflected on its synonyms: exactness, correctness, precision. Staying more in the EOLSS context we would rather consider the case of measurements distinguishing **direct** and **indirect** measurements. Direct measurements are accomplished either by counting the number of some events within a given time interval (as for instance, for Geiger counter), or by comparing a measured object with a standard, i.e. its accuracy can be evaluated quantitatively in units of a minimal scale factor. However in contemporary sciences and technologies direct measurements inhere in the lowest level of a procedure of more sophisticated indirect measuring of an observable phenomenon. Such phenomena are described, as a rule, by theoretical models with given quantitative characteristics of parameters. Thus indirect measurements suppose to be a subject of calculations that leads to the problem of the accuracy estimation from the set of measured values. This problem is caused not only by a complexity of a functional dependence connecting a chosen model, its parameters and measurements, but mainly, due to errors of latter. These errors are inherent in any measurement, direct or indirect, regardless of the thoroughness, with which the measurements have been done. The accuracy of parameters in question is inversely proportional to those errors. Therefore they have to be classified according to their sources and analysed in order to be decreased as much as possible.

There are several types of errors distinguished depending either on their sources - such as **instrumental** and **model errors**, or on their statistical behaviour - such as **bias** and **random errors**.

Instrumental errors appear due to inevitable distortions introduced to the measurements by various misadjustments of a measuring device while its construction or by misalignments of its parts. Such errors can be observed in the process of a special calibration procedure, when an especially designed standard object is measured. Results of these calibration measurements are then handled to be compared with well known features of the standard. Such calibration data handling has twofold goals: (1) to evaluate and approximate distortions of the measuring device in order to compensate them mathematically; (2) to determine a functional transformation from the scales of measuring device to the standard coordinate system. From mathematical point of view calibration problems belong to the more general class of unfolding problems described below.

Model errors are specific for hierarchical, indirect measurements and can often result in more serious errors in interpretation of experimental data. As soon as one tries to describe a certain phenomenon by a functional dependence on measured data and some parameters, then the choice of the type of function and values of its parameter can appear critical in verifying of such a description. We include here also errors of the method implementation, such as errors of approximation, rounding-up and discarding of expansion members of the higher order of smallness. A typical example of such model errors appears when one tries to approximate observations of an unknown dependence by a polynomial. A wrong choice of this polynomial degree leads to an unavoidable approximation error. It is just the error of the wrong model and results usually in a dramatic accuracy loss.

However, all the errors listed above are developed in statistics of observations and, therefore, each of them can be classified statistically either as a bias (systematic) or as a random error.

The systematic errors are caused by factors acting identically during the whole measuring process. The easiest example is weighing with a

wrong weights. It would always give you a wrong result unless you weigh a well-known standard weight, i.e. you make a calibration of your balance by calculating the difference between the previous biased measurement and the a priori known weight of your standard. Then you can weigh any object and obtain its correct weight by adding that difference to the result of this biased weighing, which is, in fact, an example of the alignment transformation.

The random errors are varying even for completely identical conditions of measurements depending on many occasional reasons which influences can not be taken into account in advance. We do not consider here rough blunders of measurements that usually can be avoided by a careful experiment design or be eliminated later by a corresponding cut-off procedure.

Thus depending on the measurement process of any experiment. some of errors listed above must be taken into account in order to improve the accuracy of measurements by a correct choice of statistical procedures embodying data handling algorithms.

2 Mathematical formalism

In mathematical formulation we have a set of measurements (a sample)

$$x_1, x_2, \ldots, x_n \tag{1}$$

to be processed statistically to extract the maximum of useful information related to the explored phenomenon with an acceptable level of accuracy. If our sample consists of equally distributed, independent random variables, then the first problem is usually to estimate their mean value and variance. More sophisticated problem is to estimate either the cumulative distribution function of our sample or its probability density function (p.d.f.). Depending on the nature of data and our *a priory* knowledge it can be done by several ways.

2.1 Distribution-free methods

If the type of the sample distribution is unknown, one of **distribution-free methods** can be applied to estimate the sample mean value and even the distribution law of our sample. Theses methods are usually based on the **order statistics** $x_{(i)}$ obtained from (1) by reordering the sample in ascending order, so that $x_{(1)} \leq x_{(2)} \leq \ldots, \leq x_{(n)}$ and the ordered measurements $x_{(i)}$ are called the order statistics. In particular, one of those statistics, namely $x_{(n/2)}$ named **the median** is a good estimation of the distribution mean value.

The *empirical probability distribution function* of the order statistics defined as

$$F_n(x) = \begin{cases} 0 & x < x_{(1)} \\ i/n & x_{(i)} \leq x < x_{(i+1)} \\ 1 & x_{(n)} \leq x \end{cases} \tag{2}$$

can serve as a good estimation of the sample distribution law, which accuracy is increased asymptotically with growing of n. That allows to determine the type of the sample distribution by some of distribution-free **goodness-of-fit test** in order to apply afterwards one of parametric methods described in the next subsection.

2.2 Parameter estimation

In a parametric case the type of the sample distribution is known and the problem is to estimate its parameters. Given the sample (1), estimation consists in determining either a value (so-called point estimation) or an interval most likely including the unknown parameter value in question (interval estimation).

2.2.1 Point estimators

Both terms: *estimation* and *estimator* are often used. There is minor difference between them: the first one is every so often denoted the process or the procedure of the parameter estimation whereas the sec-

ond one is more often denoted the specific function of the sample data which is used for parameter estimation. We shall use both terms.

Estimators are constructed as functions of our sample data and, therefore, are random values, which accuracy related properties can be expressed in probability terms only: its mean value, variance and a probability of a big deviation from the estimated parameter. Thus, having chosen an estimator, one can consider its goodness in terms of following basic properties:

- consistency,
- unbiasedness,
- efficiency,
- robustness.

An estimator is called *consistent* if its estimates converge towards the true value θ of the unknown parameter as the number n of measurements increases. The convergence is understood *in probability*, i.e. given any ε and any η, $\hat{\theta}_n$ is a consistent estimator of θ if an N exists such that

$$P(|\hat{\theta}_n - \theta| > \varepsilon) < \eta$$

for all $n > N$. One of the most widely known estimator of the center of the sampling distribution is the *arithmetic mean* of the sample data (we call it further *the sample mean*)

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i. \tag{3}$$

Its consistency follows from the famous *law of large numbers* for the majority of distributions. Although as a function of random measurements the sample mean is a random variable, it is more precise than any of these measurements, since its variance is in $\sqrt{n}$ times smaller.

It should be borne in mind that there are distributions for which the law of large numbers is incorrect and the arithmetic mean is inconsistent estimator for these distributions. As an example, consider the probability density function of the Cauchy distribution

$$p(x) = \frac{1}{\pi(1+x^2)}, \quad -\infty < x < \infty\,. \tag{4}$$

Both the mean value and the variance do not exist for the Cauchy distribution.

Denoting by E the *mathematical expectation* of a random variable we define the *bias* b of the estimator $\hat{\theta}_n$ as the deviation of its expectation from the true value θ_0,

$$b_n(\hat{\theta}_n) = E(\hat{\theta}_n - \theta_0).$$

Thus, an estimator is *unbiased* if for all n and θ_0

$$b_n(\hat{\theta}_n) = 0$$

or

$$E(\hat{\theta}_n) = \theta_0.$$

Let us take as an example such an important characteristic of any distribution as its variance, i.e. the expectation of squared deviations of a random variable from its mean

$$\sigma_x^2 = E(x - E(x))^2.$$

Calculating the *sample variance* one should replace the unknown value of the distribution mean by its statistical analog, i.e. the sample mean (3) that gives

$$S_x^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2, \tag{5}$$

which is, in fact, an estimation of the variance of our sampling distribution. However the replacement we made introduces a bias in this estimator. As it is easy to calculate, its expectation is equal to

$$E(S_x^2) = \frac{n-1}{n}\sigma_x^2 = \sigma_x^2 - \frac{1}{n}\sigma_x^2,$$

that means we have the bias term σ_x^2/n. The estimator (5) is consistent. and the presence of the small bias is not important when the sample size n is very large, but for small n we have to correct our estimator to make it unbiased

$$\tilde{S}_x^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2.$$

Two above properties are important, but not enough to describe a goodness of an estimator. Since it is a random variable, its precision can be evaluated in terms of its variance. For instance, from two above mentioned consistent estimators of the distribution center, namely the median and the arithmetic mean of the sample data, the second one has its variance smaller than for the median (in the majority of cases, when the variance of the sampling distribution does exist). The arithmetic mean can be clearly considered as the more efficient estimator than the median.

Thus in general, the *efficiency* of an estimator is determined by its variance: as it is smaller as more efficient is this estimator.

The estimator *robustness* means it should be independent of the distribution, or insensitive to departure from the assumed distribution. It such a sense the median is more robust estimation for the sample distribution center than the sample mean (3), especially for distributions like Cauchy distribution (4) one having no mean value at all.

More detailed consideration of robust estimates is given in section 3 below.

Choosing a good estimator one can note a conflict between efficiency and robustness requirements. It is typical situation when one wants to choose an estimator which must meet all requirements stated above and even some more needed to satisfy such a realistic demands as minimum computer time or a simplicity in understanding and, in general, minimum loss of scientists' time. To find a compromise one must establish an order of importance between these requirements taking into account statistical and other merits, like cost or time (urgency of completing a research). In frames of our present considerations we focus ourselves further on statistical merits.

From this standpoint one of the most powerful statistical methods for estimating parameters is the *maximum likelihood method* (MLM) invented by R.Fisher (1912). Suppose for the sample (1) we know a probability density function $f(x, \Theta)$ common for each x_i with unknown

parameter vector $\Theta = (\theta_1, \ldots, \theta_m)$. Then so-called **likelihood function**

$$L(\Theta) = \prod_i^n p(x_i). \tag{6}$$

is the density function for obtaining this sample if Θ is fixed. The MLM consists in finding an estimate of parameters $\hat{\Theta}$, which maximizes $L(\hat{\Theta})$. Since the maximum of L is also the maximum of $\ln L$, it is easier to maximize the latter function by solving *the likelihood equations*

$$\frac{\partial \ln(L(\hat{\Theta}))}{\partial \theta_k} = 0, \; k = 1, 2, \ldots, m \tag{7}$$

in order to obtain *the likelihood estimation* $\hat{\Theta}$. Its remarkable properties as *asymptotic consistency, efficiency* and *normality* are proven.

Now one can easily find MLM-estimates for a known sample distribution.

Example 1. The Gaussian distribution

$$f(x; a, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-a)^2}{2\sigma^2}\right) \tag{8}$$

For the sample (1) taken from a normal population one obtains

$$\ln(L(a, \sigma)) = -n\ln(\sigma) + \ln(2\pi^{n/2}) - \frac{1}{2\sigma^2}\sum_i (x_i - a)^2 \tag{9}$$

The solution of the likelihood equations gives two MLM-estimates

$$\hat{a} = \frac{1}{n}\sum_{i=1}^n x_i, \qquad \hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^n (x_i - \hat{a})^2, \tag{10}$$

which we already had before.

Example 2. The Poissonian distribution. It is a discrete distribution of the random variable taken value equals to a whole positive number k with the probability

$$p_k = \frac{\lambda^k}{k!} e^{-\lambda}. \tag{11}$$

For the sample $k_1, \ldots, k_n$ one has

$$\ln(L(\lambda)) = -\lambda n + \ln(\lambda) \sum_{i=1}^{n} k_i + \ln\left(\prod_{i=1}^{n} \frac{1}{(k_i)!}\right). \tag{12}$$

The solution of the likelihood equation gives the estimate of the parameter λ

$$\hat{\lambda} = \frac{1}{n} \sum_{i=1}^{n} k_i.$$

2.2.2 Interval estimators

Each of point estimators discussed above gives us a value intended to estimate an unknown parameter. As it was pointed out, these estimators are random by their nature, but obtaining a value we don't feel that its randomness is concealed and it could deceive about its accuracy or a probability of being close enough to an unknown parameter. Therefore experimenter prefers to use the estimators that include explicitly the range

$$\theta_a \leq \theta \leq \theta_b,$$

which contains the true value θ_0 with probability β. Given a measurement x from a p.d.f. $f(x|\theta)$ with a known parameter θ, the probability content β can be calculated as

$$\beta = P(a \leq x \leq b) = \int_a^b f(x|\theta)dx. \tag{13}$$

However in our case we have an unknown parameter and too large arbitrariness in choosing the interval borders a and b. It would be better to choose an interval which has minimal length among all intervals $[\theta_a, \theta_b]$ with the same probability β. Such intervals are called *confidence intervals* for θ *with probability* β. Since the parameter θ is unknown, one has to take a different variable $z = z(x, \theta)$, a function of the measurement x and the parameter θ, but such that its p.d.f. is independent of the unknown θ. If it can be found, we can re-express Eq.(13) as a problem

of interval estimation: given β, find the optimal range $[\theta_a, \theta_b]$ in θ-space such that

$$P(\theta_a \leq \theta_0 \leq \theta_b) = \beta. \tag{14}$$

It is better to explain this scheme on a particular example of the confidence interval for the mean of normally distributed sample data with the cumulative distribution function

$$\Phi(x) = \frac{1}{\sigma\sqrt{2\pi}} \int_{-\infty}^{x} \exp\left(-\frac{t^2}{2\sigma^2}\right) dt. \tag{15}$$

When both distribution parameters μ and σ are known one can calculate β from (13):

$$\beta = \Phi\left(\frac{b-\mu}{\sigma}\right) - \Phi\left(\frac{a-\mu}{\sigma}\right).$$

However when μ is unknown (but σ is known), one can instead calculate the probability β that some of functions of our measurements, say the sample mean $\bar{x}$, lies in an interval that includes its unknown mean. Let us take a symmetrical interval $[\mu - c, \mu + c]$. Then

$$\beta = P(\mu - c \leq \bar{x} \leq \mu + c) = \frac{1}{\sigma^*\sqrt{2\pi}} \int_{\mu-c}^{\mu+c} \exp\left(-\frac{(t-\mu)^2}{2\sigma^{*2}}\right) dt =$$

$$= \Phi\left(-\frac{c}{\sigma^*}\right) - \Phi\left(\frac{c}{\sigma^*}\right), \tag{16}$$

where for the sample mean $\sigma^* = \sigma/\sqrt{n}$. We can now invert the probability statement in (16) in order to take the form of the statement (14):

$$\beta = P(\bar{x} - c \leq \mu \leq \bar{x} + c).$$

As it is known in the case of the normal distribution, one can obtain $\beta = 0.95$ if the constant c is chosen as

$$c = 1.96\,\sigma^* = 1.96\,\sigma/\sqrt{n}.$$

2.3 Evaluation of dependencies

Now we consider more complicate set of two-dimensional observations

$$(x_1, y_1), \ldots, (x_n, y_n) \tag{17}$$

which we want to describe by a known function f embodying our model assumption by means of parameters in question $\theta_1, \theta_2, \ldots, \theta_m$. It gives us the following system of equations

$$y_i + e_i = f(x_i; \theta_1, \theta_2, \ldots, \theta_m), \quad i = 1, 2, \ldots, n, \tag{18}$$

where e_i are the errors of measurements., which supposed to be random variables all with the zero mean values and common distribution function $F_e(x)$; n is a number of measured points.

For the easiest 2D-case the equations (18) can be considered as the set of residuals between the measured points and a curve to be fitted to them by varying the vector $\bar{\Theta}(\theta_1, \theta_2, \ldots, \theta_m)$:

$$e_i = y_i - f(x_i; \bar{\Theta}), i = 1, 2, \ldots, n. \tag{19}$$

where x_i is a given abscissa of the i-th measurement y_i.

2.3.1 Least squares and maximum likelihood

The least squares method (LSM) was independently invented by C.F.Gauss (1805) and A.Legendre (1809) and it consists in **minimizing of the sum of squares of those residuals** (19)

$$S(\bar{\Theta}) = \sum_{i=1}^{n} \left(y_i - f(x_i; \bar{\Theta})\right)^2 \tag{20}$$

in respect to unknown parameters. Since $S(\bar{\Theta})$ is a quadratic function of its arguments, its minimum is reached when all $\partial S / \partial \theta_k = 0; k = 1, 2, \ldots, m$ hold. This system of equations is especially simple in the mostly used case of the linear regression:

$$f(x_i; \bar{\Theta}) = \sum_{j=1}^{m} \phi_j(x_i) \cdot \theta_j + e_i, \quad i = 1, \ldots, n, \tag{21}$$

where $\phi_j(\cdot)$ is known set of m linearly independent basic functions (e.g. $1, x, x^2, \ldots, x^m$); e_i - an accidental measurement errors; θ_j are as above unknown regression parameters ($j = 1, \ldots, m$) which should be estimated by use of our data sample. Then the equation system for parameter estimations becomes linear. It called **the normal system of equation.**

Optimal properties of LSM curve fitting follow from the fact that LSM is a particular case of the more general maximum likelihood method. As in section 2.2.1 under the assumption that all residuals (19) are independent random variables with zero mean and a common p.d.f. $p(e)$ one has the probability of occurring of our particular sample $e_1, e_2, \ldots, e_n$, is equal to likelihood function

$$L(\bar{\Theta}) = \prod_i^n p(e_i). \tag{22}$$

Then we choose as the likeliest estimation of parameters the value of $\bar{\Theta}$ in which (22) has its maximum. The solution of the likelihood equation

$$\frac{\partial \ln(L(\bar{\Theta}))}{\partial \theta_k} = 0,\ k = 1, 2, \ldots, m \tag{23}$$

gives the likelihood estimations $\hat{\bar{\Theta}}$. Under the crucial assumption of normality of the p.d.f. in (22), i.e.

$$p(e_i) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{e_i^2}{2\sigma^2}\right), \tag{24}$$

one immediately has that MLM converts to LSM. Since

$$\ln(L(\bar{\Theta})) = \ln\left(\prod_{i=1}^n p(e_i)\right) = \sum_{i=1}^n p(e_i),$$

the logarithmic likelihood function becomes equal to

$$-\frac{1}{2}\sum_{i=1}^n \left(\frac{e_i^2}{\sigma^2}\right) + \text{const},$$

which has its maximum exactly at the same point where (20) has its minimum. This implies that all above-mentioned good properties of a LSM-estimation are valid only if the normality assumption holds.

2.3.2 Measurements with different accuracy

Again we assume that the errors of measurements are distributed normally about zero, i.e.

$$y_i = f(x_i; \bar{\Theta}) + e_i,\ E(e_i) = 0,\ E(e_i^2) = \sigma^2 = 1/w_i.$$

The LSM requires

$$S = \sum_{i=1}^{n} w_i e_i^2 \Longrightarrow \mathbf{min}. \tag{25}$$

The terms in the sum of squares are now *weighted* by the reciprocals of the variances. We explain details of S minimization for the linear case (21) with $\phi_j(x_i) = x_i^{j-1}$ in the following notations

$$\mathcal{X} = \begin{pmatrix} 1 & x_1 & x_1^2 & \ldots, & x_1^m \\ 1 & x_2 & x_2^2 & \ldots, & x_2^m \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \ldots, & x_n^m \end{pmatrix},\ \mathcal{Y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix},\ \Theta = \begin{pmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_m \end{pmatrix}.$$

Defining also the weight matrix

$$\mathbf{W} = \begin{pmatrix} w_1 & & & 0 \\ & w_2 & & \\ & & \ddots & \\ 0 & & & w_n \end{pmatrix}$$

we can rewrite (25) in its matrix form as

$$L = \mathcal{E}^T \mathbf{W} \mathcal{E},$$

where $\mathcal{E} = \mathcal{Y} - \mathcal{X}\Theta$. Then the solution of the normal system of equations becomes

$$\hat{\Theta} = (\mathcal{X}^T \mathbf{W} \mathcal{X})^{-1} \mathcal{X}^T \mathbf{W} \mathcal{Y}$$

It gives us estimations of all $m+1$ parameters of our fit. Their covariance matrix is

$$\mathrm{cov}(\hat{\Theta}) = \mathcal{C} = (\mathcal{X}^T \mathbf{W} \mathcal{X})^{-1}.$$

It contains squared errors of parameters on its diagonal, but since those parameters are correlated, one can obtain also covariances of i-th and j-th parameters as the element c_{ij} of this matrix.

3 Robust approach

Actually, the crucial normality assumption is very often violated due to contamination of the measurements by points of noise or background. Then due to quadratic view of the functional S in (20) the contribution to it of any sample point-outlier could seriously disturbs the estimations of parameters that causes a dramatic loss of accuracy. To calculate correct values of parameters one should use only the measurements from a close vicinity of the fitted function $f(x;\bar{\Theta})$. All others should have much less impact or be completely negligible. This idea can be implemented by attributing **special weights** to each of measurements. Values of these weights must decrease with the growth of residuals e_i, i.e. of the distance from the fitted curve. This approach named **robust**, i.e. resistive to contamination, has been proposed by P.Huber (1972). Let us take as an example a linear regression dependence (21) to expound how to find the best way to process the noisy data by such a robust approach.

We describe the contaminated distribution of measurement errors e_i by J.Tukey's *gross-error model*

$$f(e) = (1-\beta)\cdot p(e) \; + \beta \cdot h(e) \; , \tag{26}$$

where β is a parameter of contamination, $p = N(0,\sigma_m^2)$ is the Gauss distribution (24), and h is some long-tailed noise distribution. Using the maximum likelihood method

$$L = \prod_{i=1}^{N} f(e_i) \Longrightarrow \mathbf{max}$$

we obtain the following system of non-linear equations

$$\sum_{i=1}^{N} w_i \cdot \left(Y_i - \sum_{j'}^{p} \phi_{j'}(x_i)\cdot\theta_{j'} \right) \cdot \phi_j(x_i) = 0 \tag{27}$$

with some optimal weights w_i depending on relations of p and h distri-

butions

$$w_i = \frac{p(e_i)}{p(e_i) + \dfrac{\beta}{1-\beta} \cdot h(e_i)}. \tag{28}$$

Taking $p(e)$ from (24) and $h(e)$ to be uniform and equals $h = h_0$ for. distinctness one obtains the optimal weight function as

$$w_{opt}(e) = \frac{1+c}{1 + c \cdot \exp\left(\dfrac{e^2}{2}\right)}, \tag{29}$$

with the constant

$$c = \frac{h_0 \beta \sigma \sqrt{2\pi}}{1-\beta}.$$

These weights are non-linear functions of parameters in questions. Therefore an iterative procedure was elaborated, in which the weights are recalculated on each iteration in accordance with the new values of parameters. This procedure is referred as re-weighted LSM (RWLSM). A polynomial expansion of these optimal weights up to the fourth order leads to the approximation

$$w(t) = \begin{cases} \left(1 - (t/c_T)^2\right)^2, & \text{if } |t| < c_T \\ 0\,, & \text{otherwise.} \end{cases} \tag{30}$$

We obtain, in fact, the famous Tukey's bi-weights which are easier to calculate than optimal ones. It is also recommended to choose the cutting parameter $c_T = (3 \div 4)\sigma$. If there is no *a priori* information one can initiate the iterations with $w_i^{(0)} = 1$.

The parameter σ should be also recalculated on each iteration

$$\sigma^{(k)} = \sqrt{\frac{\sum\limits_i w_i^{(k-1)} \left(e_i^{(k-1)}\right)^2}{\sum\limits_i w_i^{(k-1)}}} \tag{31}$$

Following P.Huber one can consider this procedure as descending M-estimate. Thus the robust approach allows to handle data accurately

even in presence of contamination, but if one is sure that data to be processed are free from background, noise or other contaminating factors, then there is no need to use any RWLSM-procedure, since the LSM is proven to be the most efficient method in this case.

4 Resolution of digitized signals

It should be noted, however, at this point that the situation with real measurements in majority of contemporary physical, chemical or biological experiments is much far from the idealized models described above. Almost any modern measuring device is a quite sophisticated physical apparatus, which registers results of measurements in a discrete form after a digital procedure. In order to improve the resolution and accuracy of such detectors, they are designed as granular structures consisting of an array (raster) of cells (pads). Therefore if a signal to be detected looks like a single thin peak after being registered it would be smeared by the measuring device between several adjacent cells and then it is discretized in a view of a histogram, which dimension depends on experimental data. An accidental measurement error is added to each histogram bin during registration. Additionally, background noise gives also its contribution to every cell of our device raster.

The basic problem is: to reconstruct the original signal position and its other parameters (its amplitude or the volume under its surface, its half-width etc) from the registered histogram. Depending on its formulation this problem can be solved in either non-parametric or parametric ways.

4.1 Non-parametric approach

The first non-parametric approach also named *the unfolding problem* is applied when the parametrization of the problem is unknown. Taking one-dimensional case for simplicity one can present a measurement result as one-dimensional histograms $\{F_i\}$ for $i = 1, 2, \ldots, n$. which bin sizes and centers we denote correspondingly as Δ_i and x_i. These

measured values are distorted by the detector influence and spoiled by noise. We assume that the values of the random function $F_i = F(x_i)$ are independent at different x_i and they do not contain systematical errors. Let us denote by $K(x,y)$ the instrumental or the point spread function of our detector. In the most cases it is symmetrical and depends only on the difference of its arguments, i.e. $K(x,y) = K(x-y)$ as, for instance, a Gaussian

$$K(s) = \exp\left(-\frac{s^2}{2{\sigma_s}^2}\right)$$

with σ_s usually supposed to be a known constant. Then one can, in principle, reconstruct the original signal in question $f(x)$ as a solution of the system of following integral equations of the first kind

$$F_i = \int\limits_{\Delta_i} K(x-y)f(y)dy = \int\limits_{x_i-\Delta/2}^{x_i+\Delta/2} K(x-y)f(y)dy,\ i = 1,2,\ldots,n\,. \quad (32)$$

The finite size Δ of the detector granularity can be expressed as the function $h(x)$

$$h(x) = \begin{cases} 1, & |x| \le \Delta/2 \\ 0, & |x| > \Delta/2\,. \end{cases} \quad (33)$$

It allows to take into account the signal distorsions due to the histogramming process of the experimental data storing. Its influence can be expressed mathematically by convolution of the point spread function $K(s)$ with the granularity function $h(x)$ giving the modified instrumental function

$$K_1(s) = \int h(s-r)K(r)dr\,. \quad (34)$$

Therefore the system (32) is transformed to

$$F_i = F(x_i) = \int K_1(x_i - x)f(x)dx. \quad (35)$$

Due to discreteness of our model the integral equation system (35) is reduced to the system of algebraic equations suitable for implementing

by computer

$$\sum_{j=1}^{m} P_{ij} G_j = F_i, \; i = 1, 2, \ldots, n, \tag{36}$$

where $G_j = f(y_j)$ are unknown variables and

$$P_{ij} = K_1(x_i - y_j) \cdot (y_{j+1} - y_j). \tag{37}$$

Unfortunately in most cases the system (36) is ill-posed, i.e. it has no solution at all since its right-hand side is a random vector and the system matrix P_{ij} is practically degenerated. However as it can be proved, when one looks for a solution on a compact set, the problem can be solved for a sufficiently wide class of kernels including the convolution $K_1(s)$.

In the case of Gaussian distribution function of input data the logarithmic likelihood function may be written as

$$L = -\frac{1}{2} \sum_{i=1}^{n} \frac{(F_i - S_i)^2}{\sigma_i^2} + \text{const}, \tag{38}$$

where σ_i^2 are the noise variances at the i-th experimental point and the values of S_i are defined by the formula

$$S_i = \sum_{k=1}^{m} P_{ik} G_k, \quad i = 1, 2, \ldots, n.$$

The sought maximum of the likelihood function L can be calculated by by means of an iterative procedure. As it has been proved by E.L.Kosarev (1993), this procedure converges to the maximum of the likelihood function (38).

E.L.Kosarev has also shown (1990) that the resolution obtained reaches the possible theoretical limit. Such a limit for close signals follows from the well-known Shannon's theorem for the maximum speed of the data transmission via the channel having a noise. The **resolution** of any linear device with the instrumental function $K(x)$ can be defined as the effective width of this function, i.e.

$$D = \int_{-\infty}^{\infty} K^2(x) dx, \tag{39}$$

providing the normalizing condition at the origin $K(0) = 1$.

The resolution of spectral devices can be improved in comparison to D using the modern techniques for solving integral equations, thus **superresolution** is achieved. We define **the superresolution factor** as the ratio of D to the separation δ between two narrow lines which can be recovered after the deconvolution procedure

$$SR = D/\delta \ . \tag{40}$$

We should remind that according to the well-known Rayleigh's definition of resolution $\delta = D$, so in this case the superresolution factor is $SR = 1$. When the resolution is improved mathematically, $SR > 1$. The improvement is always limited by noise. At zero noise an exact solution of Eq.(35) can be found, which corresponds to an infinite superresolution.

The highest possible superresolution factor is closely related to the Shannon theorem on the highest possible transmission rate of information through a noisy channel. When a spectrum is not parametric, i.e. the function we sought for cannot be described by a simple formula with a few parameters, the limiting superresolution factor is

$$SR = \frac{1}{3}\log_2(1 + E_s/E_n). \tag{41}$$

Here E_s and E_n

$$E_s = \int_{-\infty}^{\infty} F^2(x)dx, \ E_n = n\sigma^2,$$

are the signal energy and the noise one. Here n is the number of experimental data points, and σ^2 is the variance of input noise. If the signal-to-noise ratio is expressed in decibels $dB = 10\log(E_s/E_n)$, the approximate expression for the superresolution limit is

$$SR \simeq dB/10. \tag{42}$$

The computer program package RECOVERY was described, which can reach the Shannon superresolution limit.

4.2 Parametric approach

The second parametric approach is well-known as parameter fitting. It is obvious that parametric methods must be more accurate than non-parametric ones, since the parametrization itself brings an essential information related to processed signals. Even such a general knowledge as the signal symmetry is enough to apply the easy-to-calculate center of gravity (COG) method for estimation of the signal centroid:

$$x_{cog} = \frac{\sum\limits_i a_{i,j}\bar{x}_i}{\sum\limits_i a_{i,j}} \qquad y_{cog} = \frac{\sum\limits_j a_{i,j}\bar{y}_j}{\sum\limits_j a_{i,j}}, \tag{43}$$

where $a_{i,j}$ is 2D histogram presenting a detector response to the current signal, $\bar{x}_i, \bar{y}_j$ are the middle points of the corresponding bins. The high speed and universality of this method made it the most popular for the majority of discrete detectors, unless the signal overlapping due to the high occupancy in many of modern experimental systems. It occurs when the probability of two and more signals to be overlapped is high enough.

Therefore more elaborated methods based on LSM robust modifications are developed by G.Ososkov (1997). Due to the problem of non-linearity they are iterative, so the COG solution can be used as an initial approximation. A multiparametric model of a signal obtained as a superposition of two gaussian peaks with different positions and amplitudes is used. Corresponding problem of non-linear LSM functional minimization is solved there by a paraboloidal approximation method. As one more example of successful applications to the same problem of the close signal resolution, a method using wavelet transforms can be also pointed out. There are a great number of such examples of successful solutions of signal recovery parametric problems in different fields. All these methods have various degree of accuracy depending on the noise or contamination level, but from statistical point of view all they intend, as the matter of facts, to provide various estimations of parameters.

Thus a question arises: is there a limiting accuracy and how to reach it?

4.3 Cramér-Rao lower-bound for accuracy

For the sake of simplicity let us consider a model of estimating of the single signal location parameter x_0 from a sample of n measurements:

$$y_i = A\psi(x_i - x_0) + \varepsilon_i, \qquad i = 1, 2, .., n.$$

Here $\psi(x)$ is the signal shape, A is its amplitude, and a random noise ε_i has the Gaussian distribution $N(0, \sigma)$, i.e.

$$p(\varepsilon_i)d\varepsilon_i = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{\varepsilon_i^2}{2\sigma^2} \right] d\varepsilon_i \ ,$$

where different noise sample units are assumed to be (for a simplicity again) independent and non-correlated: $\overline{\varepsilon_i \varepsilon_j} = \sigma^2 \delta_{ij}$. Applying the standard maximum likelihood method for estimating the signal amplitude A and location parameter x_0 one has to maximize the likelihood function of the sample

$$L = \prod_{i=1}^{n} p(\varepsilon_i) = \left(\frac{1}{\sqrt{2\pi}\sigma} \right)^n \exp\left[-\frac{1}{2\sigma^2} \sum_{i=1}^{n} \varepsilon_i^2 \right] =$$

$$= \left(\frac{1}{\sqrt{2\pi}\sigma} \right)^n \exp\left[-\frac{1}{2\sigma^2} \sum_{i=1}^{n} [y_i - A\psi(x_i - x_0)]^2 \right].$$

It reduced to maximizing the logarithmic likelihood function

$$l = \ln L = \text{const} - \frac{1}{2\sigma^2} \sum_{i=1}^{n} [y_i - A\psi(x_i - x_0)]^2 \ .$$

According to the Cramér-Rao inequality *for unbiased estimates* one has

$$D(x_0) \geq \frac{1}{E\left[\left(\frac{\partial l}{\partial x_0} \right)^2 \right]} \ .$$

Here, as usually, the symbol E denotes the mathematical expectation obtained by various random realizations of ε_i for $i = 1, 2, \ldots, n$. Taking the partial derivatives with respect to the parameter x_0 one obtains the following formula for the Cramér-Rao lower-bound for the accuracy of the signal location parameter x_0 under condition of the negligible correlation between x_0 and A

$$D(x_0) \geq \frac{\sigma^2}{A^2} \cdot \frac{1}{\sum_{i=1}^{n} \left[\frac{\partial \psi(x_i - x_0)}{\partial x_0} \right]^2} \cdot \tag{44}$$

This final formula is valid for arbitrary shapes of the signal $\psi(x)$ and arbitrary ratio between the characteristic scale D of the function $\psi(x)$ and the bin size Δ (the latter can be treated as the distance between measured points).

Let us consider two limiting cases. In the first one when $\Delta \ll D$, the Eq.(44) can be approximated by substituting of the sum in denominator by the corresponding integral

$$\Delta \cdot \sum_{i=1}^{n} \left[\frac{\partial \psi(x_i - x_0)}{\partial x_0} \right]^2 \approx \int_{-\infty}^{\infty} \left(\frac{\partial \psi}{\partial x} \right)^2 dx. \tag{45}$$

Here Δ denotes the histogram bin size. Computing the corresponding integral for the signal shape $\psi(x) = \exp(-(x/D)^2)$ one obtains eventually the formula

$$D(x_0) \geq \frac{\sigma^2}{A^2} \cdot \frac{1}{\sum_{i=1}^{n} \left[\frac{\partial \psi_i}{\partial x_0} \right]^2} \approx \frac{\sigma^2}{A^2} \cdot \frac{D\Delta}{\sqrt{\frac{\pi}{2}}}$$

and its approximate estimation

$$\delta x_0 = \sqrt{D(x_0)} \approx \frac{\sigma}{A} \cdot \frac{\sqrt{D\Delta}}{(\pi/2)^{1/4}} \approx 0.89 \frac{\sigma}{A} \sqrt{D\Delta}. \tag{46}$$

If $\sigma/A = 5\%$, $D = 4$, $\Delta = 1$, one has $\delta x_0 \approx 0.1$, i.e. 10 times better than bin size.

In the second limiting case both characteristics scales D and Δ are approximately of the same size

$$D \sim \Delta.$$

In this case the approximation Eq.(45) is not valid and one should compute explicitly the sum in the denominator of the Eq.(44).

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5 Glossary

- ## Bias

  Bias $b(\theta)$ in statistical terminology is determined as the deviation of the mathematical expectation E of some estimation T_θ of a parameter θ from the true value of this parameter

  $$b(\theta) = E(T_\theta) - \theta.$$

  If $b(\theta) \equiv 0$ then the estimation T_θ is **unbiased**.

- ## Distribution function

  Distribution function (often: cumulative distribution) $F(t)$ of some random variable $\mathbf{x}$ is determined as the probability P of the event that $\mathbf{x} < t$

  $$F(t) = P(\mathbf{x} < t), \ -\infty < t < \infty.$$

  The function $F(t)$ is non-decreasing and continuous from the left.

- ## Error

  Error ε of a measurement x of some value x_0 is usually determined as deviation of the result of the measurement x from the value of x_0

  $$\varepsilon = x - x_0.$$

  There are two kinds of errors: random and bias and both are essential as a contribution to the final accuracy of measurements. There is a lower limit of any accuracy achievable by data handling based on the Cramér-Rao theorem.

- ## Estimation

  Estimation is in a general case a function f of measurements $x_1, \ldots, x_n$ and it is therefore a random variable. The value of this function $f(x_1, \ldots, x_n)$ is *an estimation* of unknown characteristic - the latter one can be a set of parameters or a distribution function.

- ## Least squares

  Least squares is a parameter estimation method which consists of minimizing the sum of squared deviations of the data $y_i, i = 1, \ldots, n$ of

the measurements from some function $y(x; a_1, \ldots, a_m)$ of x-coordinate to be fitted by a proper choice of unknown parameters $a_1, \ldots, a_m$

$$S = \sum_{i=1}^{n} (y_i - y(x_i; a_1, \ldots, a_m))^2 \Longrightarrow \mathbf{min}.$$

If measurements y_i, $i = 1, \ldots, n$ have the Gauss distribution the Least Squares Method (LSM) is a particular case of the **Maximum Likelihood Method** (MLM).

- ## Likelihood

Likelihood function

$$L(t|\theta) = L(t_1, \ldots, t_n|\theta_1, \ldots, \theta_m)$$

is determined as the probability that measurements $x_1, \ldots, x_n$ are taken fixed values $t_1, \ldots, t_n$. This definition is valid only for discrete variables x_i. In continual case one must replace 'probability' to 'probability density'. According to the MLM one can find the values of unknown parameters $\theta_1, \ldots, \theta_m$ by maximization of the likelihood function in the $m-$dimensional parameter space $\{\theta_k\}$, $k = 1, \ldots, m$. The arguments of the likelihood function

$$t_i = x_i,\ i = 1, 2, \ldots, n$$

are considered as fixed while the maximization process.

- ## Parametric method

Parametric method is in fact the MLM when one looks for some unknown parameters $\theta_1, \ldots, \theta_m$ from measurements $x_1, \ldots, x_n$ under the condition that number of parameters

$$m \ll n.$$

If the last inequality does not hold, the parametric method can sometimes result in inconsistent estimations.

- ## Resolution

Resolution (sometimes denoted as **resolving power**) is determined

for any linear registering device (e.g. a spectrometer in optics) with the instrumental function $K(x)$ as

$$D = \int_{-\infty}^{\infty} K^2(x)dx,$$

providing the normalizing condition $K(x_0) = 1$ where x_0 is the abscissa point where $K(x_0) = \max$. The resolution of a registering device can be improved in comparison with D by applying the modern techniques for data treatment, thus **superresolution** can be achieved.

- ## Robust approach

Robust approach is a way of statistic estimation design to be less sensitive to disturbance of the basic hypotheses concerning the data and contaminating noise.

- ## Sample

Sample of the size n is a set of elements

$$x_i,\ i = 1, \ldots, n$$

randomly chosen from a general population, i.e. another set of elements $\{\xi\}$ of infinite size with the distribution function $F(\xi)$. According to this definition elements $x_i,\ i = 1, \ldots, n$ are equally distributed, independent random variables. It should be mentioned that experimentalists prefer usually to say: "data" instead of "sample", "measure" instead of "draw a sample", and "observable space" instead of "general population".

- ## Statistics

Statistics in context of this article is the one of two connected parts of the mathematical science "Probability theory and mathematical statistics". Mathematical statistics is more 'experimental' science with comparison of a probability theory, because we have to draw information from the experimental data. We can consider problems of both theories as direct and inverse.

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Ососков Г. А., Косарев Е. Л.
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Допуски и точность при измерениях

На основе теории вероятностей и математической статистики излагаются методы определения предельно достижимой точности измерений. Обсуждаются непараметрические и параметрические методы, точечные и интервальные оценки неизвестных параметров. Показано соответствие между методом максимального правдоподобия и методом наименьших квадратов. Специальный раздел посвящен робастным оценкам и способам разрешения близких оцифрованных сигналов. Показано, как неравенство Крамера–Рао определяет нижнюю границу точности измерений.

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Ososkov G. A., Kosarev E. L.
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Limits and Accuracy in Measurements

Methods of determination of the limit attainable accuracy in measurements are expounded on the basis of the probability theory and the mathematical statistics. Distribution-free and parametric methods, point and interval estimations of the unknown parameters are discussed. The connection between maximum likelihood method and least squares method is shown. A special section is devoted to robust estimations and to resolution of digital signals. It is demonstrated how the Cramer–Rao inequality determines the lower-bound for the accuracy of measurements.

The investigation has been performed at the Laboratory of Information Technologies, JINR.

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