Selection of a regression model for graduation of measuring instruments when it is necessary to estimate stability of the calibration curve

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Abstract. A method for choosing the best regression model for the cases when the measuring task is associated with the study of the stability of the metrological characteristics of the calibrated measuring instrument is described. A description of the experiment set up when using this method in the course of researching the metrological characteristics of measuring instruments for the numeric concentration of light air ions is given, and the research results obtained using this method are given.

1. Introduction

The problem of choosing a regression model often arises in solving different measuring tasks. This problem is solved in various ways, depending on a specific task. The main regulatory document in the Russian Federation devoted to this problem is the recommendations R 50.2.004 [1], which establishes the principles for determining the characteristics of mathematical models in the field of state metrological control and supervision. These recommendations are based on the method of maximum compactness described in more detail in [2].

This work proposes a method for choosing a regression model for cases when the measuring task is associated with stability testing of the metrological characteristics (MC) of a calibrated measuring instrument (MI). When using polynomial models, it should be remembered that increasing the degree of the polynomial is not always desirable, since polynomials of high degrees are more sensitive to fluctuations of measurement results, therefore they may not describe the true relationship between physical values as adequately as polynomials of lower degrees. This effect is particularly pronounced when it is supposed to use the obtained characteristic in determining the instability of the MI’s MC. In this case, if a point far removed from the long-term average value falls into the input data, deviations of the measurement results from the values expected by the calibration curve will be higher on average.

The proposed method is based precisely on the effect of an apparent increase in the instability of the MC when the degree of the polynomial is too high. The method is as follows:

1. The information about the MI’s MC as a function of the value of the measured quantity is obtained experimentally.
2. By least square method, the calibration curve in various models is estimated (for example, polynomials of different degrees).
3. For each model, residual error $\delta$ is estimated by the formula:

$$\delta = \max \left| \frac{\rho_o - \rho_m}{\rho_o} \right|, \quad (1)$$

where $\rho_o$ is the reference value and $\rho_m$ is the measuring result corrected according to the obtained calibration curve.

4. After further research, the instability $\nu_p$ is evaluated according to RMG 74-2004 [3] (the method is also described in [4]). This value is also evaluated for each regression model.

5. The regression model is chosen under criterion of the smallest aggregate error $\theta$ estimated by the formula:

$$\theta = \sqrt{\delta^2 + \nu_p^2}. \quad (2)$$

This method allows to choose the best regression model and then use this particular model performing periodical calibration of the MI without studying its long-term characteristics.

The method was developed during the creation of working standards for the counting concentration of light air ions for regional centers of standardization and metrology. When creating working standards, the task arose of calibrating working standards and assessing the deviation of their metrological characteristics from the calibration values during the interval of 1 year. Below are the results of experimental research of air ion counters’ metrological characteristics as an example of the implementation of the method.

2. Description of the experiment

A light ion generator from the state standard GET 177-2010 was used to create a reference medium with a given numeric concentration of air ions. Due to the wide measuring range that covers four orders of magnitude, the measurement error of air ion counters is usually presented in the form of a relative measurement error. This form of presentation is convenient for comparing measurement errors in different ranges. During the experiment, at least two values were used in the ranges $(1 - 9.99) \cdot 10^2$ and $(1 - 10) \cdot 10^5$ ions/cc and at least one value in the ranges $(1 - 9.99) \cdot 10^3$ and $(1 - 9.99) \cdot 10^4$ ions/cc. This requirement was imposed on the basis of the practice of calibration of air ion counters, where it was noticed that the metrological characteristics of air ion counters tend to change sharply near the boundaries of the measurement subranges.

The measurements were carried out with the volumetric air flow through the reference SI at $(14.0 \pm 0.2)$ m$^3$ / h. At this value, the linear velocity of the air flow taken by the reference SI approximately coincides with the linear velocity of the air flow at the outlet of the air ion generator, which makes it possible to avoid additional errors associated with aerodynamic reasons. The tolerance was chosen based on the observed drift of the volumetric air flow during the day, as well as due to the high sensitivity of the volumetric airflow value to the angle of rotation of the control valve of the duct. The relative measurement error was determined as the relative deviation of the mean value of the readings of the calibrated meter from the mean value of the readings of the reference SI.

3. Evaluation of the metrological drift during the 1-year interval

The evaluation of the metrological drift during the 1-year interval was done by establishing the parameters of the drift of the metrological characteristics (MC) of the measuring instrument and calculating the limit of permissible values of the confidence limits of the instability of the metrological characteristics of measuring instruments depending on the calibration interval.

The probabilistic characteristics of the instrument’s MC drift process were experimentally determined from the results of measurements of the instability for time intervals equal to 1 month:

- average instability as
\[ m(T) = \frac{1}{n} \sum_{i=1}^{n} \xi(t_i) \]  

(3)

where \( \xi(t_i) \) is the instability determined in the i-th month;

- standard deviation of instability as

\[ \sigma(T) = \sqrt{\frac{1}{n-1} \sum_{i=1}^{n} [\xi(t_i) - m(t)]^2} \]  

(4)

The confidence limits for the instability of the MC SI were determined by the formula

\[ \nu_p(T) = \max \left\{ \left| m(T) - z_{0.5(1+P)} \sigma(T) \right|^{1/F}, \left| m(T) + z_{0.5(1+P)} \sigma(T) \right|^{1/F} \right\} \]  

(5)

where \( F \) is an indicator equal to 1 for a normal distribution, \( z_{0.5(1+P)} \) is the quantile of the density of the normal distribution for a confidence level of 0.5(1 + P) at \( P = 0.95 \), equal to 3.22,\( T \) is the calibration interval equal to 1 year.

4. Results

As a result of the experiment, calibration curves were obtained for two working standards, each of which included two measuring instruments, on the positive and negative measurement channels - a total of eight curves per month.

One of such characteristics is shown in Figure 1. The figure shows that the relative measurement error changes sharply in the range from \( 10^2 \) to \( 10^3 \) ions/cc. This persists with subsequent monthly calibrations, as shown in Figure 2.

![Fig. 1 Measurement error as the function of numeric concentration](image-url)
Fig. 2. Measurement error as the function of numeric concentration in monthly experiments

Thus, due to the sharp change in the character of the curve in the region of $10^3$ ions/cc, it is natural to divide the calibration characteristic into two ranges: from $10^2$ to $10^3$ cm$^{-3}$ and from $10^3$ to $10^6$ ions/cc. Since the second measurement range covers several orders of magnitude, in order to avoid excessive sensitivity of the resulting characteristic to the upper limit, it was decided to logarithm the argument in this range, i.e. the dependence $\delta$ (log ($\rho$)) was investigated.

The calibration curve was approximated by a polynomial function, and the degree of the polynomial was determined according to the principle of the least drift of the metrological characteristics during subsequent periodic calibrations. The $R^2$-criterion, usually used to select the type of regression model, was not used in this case, since for the purposes of the study it was important to evaluate the correctness of the obtained characteristic when it was used for 1 year, while the $R^2$-criterion operates only on the data on the day of calibration.

Tables 1 and 2 present the research results for two working standards. The confidence limits for the instability of the MCS were calculated using the formula (5), the non-excluded remainder of the relative measurement error using the formula

$$\delta = \max \left| \frac{\hat{\rho} - \rho_S}{\rho_S} \cdot 100\% \right|$$  \hspace{1cm} (6)

where $\hat{\rho}$ is the result of measurements corrected according to the obtained calibration characteristic, $\rho_S$ is the result of measurements of the numeric concentration on the state standard.

The total error was estimated according to the formula

$$\theta_x = \sqrt{\delta^2 + \nu_p^2}$$  \hspace{1cm} (7)

These values were calculated for polynomials of degree 0 (constant correction factor), 1, 2 and 3 in the range from $10^1$ to $10^6$ cm$^{-3}$. In the range from $10^2$ to $10^3$ cm$^{-3}$, only polynomials up to power 2 were considered due to the smaller amount of experimental data in this range. The cases for which it is minimal and which were accordingly selected for the calibration curve are highlighted in gray.
Table 1. Results for the first working standard (REKLA-1) in the range of $10^3$ to $10^6$ ions/cm$^3$

| Channel | Polarity | Degree of the polynomial |
|---------|----------|-------------------------|
|         |          | 0   | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   |
|         |          | $\delta$ | $v_p$ | $\theta_\Sigma$ | $\delta$ | $v_p$ | $\theta_\Sigma$ | $\delta$ | $v_p$ | $\theta_\Sigma$ |
| 1       | «+»      | 2.5  | 7.2 | 7.6 | 1.6 | 7.4 | 7.6 | 1.3 | 8.2 | 8.3 |
|         | «-»      | 4.1  | 6.5 | 7.7 | 2.5 | 7.1 | 7.5 | 1.5 | 7.6 | 7.7 |
| 2       | «+»      | 2.7  | 6.7 | 7.2 | 2.2 | 7.6 | 7.9 | 2.1 | 7.7 | 8.0 |
|         | «-»      | 5.9  | 7.2 | 9.3 | 4.3 | 7.9 | 9.0 | 3.8 | 8.6 | 9.4 |

Table 2. Results for the first working standard (REKLA-1) in the range of $10^3$ to $10^6$ ions/cc

| Channel | Polarity | Degree of the polynomial |
|---------|----------|-------------------------|
|         |          | 0   | 1   | 2   | 3   |
|         |          | $\delta$ | $v_p$ | $\theta_\Sigma$ | $\delta$ | $v_p$ | $\theta_\Sigma$ |
| 1       | «+»      | 1.8  | 4.1 | 4.5 | 1.6 | 4.3 | 4.6 | 1.2 | 4.4 | 4.6 | 1.1 | 5.6 | 5.7 |
|         | «-»      | 2.7  | 3.7 | 6.1 | 1.9 | 4.8 | 6.4 | 3.5 | 4.7 | 5.9 | 2.5 | 6.0 | 6.5 |
| 2       | «+»      | 4.8  | 3.7 | 6.1 | 4.5 | 6.4 | 4.3 | 5.2 | 4.7 | 5.9 | 2.5 | 6.0 | 6.5 |
|         | «-»      | 4.5  | 3.7 | 6.1 | 4.2 | 6.3 | 4.7 | 4.9 | 5.2 | 5.5 | 1.5 | 5.5 | 5.7 |

Table 3. Results for the second working standard (REKLA-1M) in the range of $10^3$ to $10^5$ ions/cc

| Channel | Polarity | Degree of the polynomial |
|---------|----------|-------------------------|
|         |          | 0   | 1   | 2   |
|         |          | $\delta$ | $v_p$ | $\theta_\Sigma$ | $\delta$ | $v_p$ | $\theta_\Sigma$ |
| 1       | «+»      | 18.5 | 9.1 | 20.6 | 7.3 | 7.6 | 10.5 | 3.4 | 10.2 | 10.8 |
|         | «-»      | 17.7 | 6.5 | 18.9 | 6.9 | 7.4 | 10.1 | 1.8 | 10.1 | 10.3 |
| 2       | «+»      | 15.9 | 6.2 | 17.1 | 4.6 | 7.0 | 8.4 | 3.6 | 8.4 | 9.3 |
|         | «-»      | 4.7  | 5.6 | 7.3 | 1.6 | 5.7 | 5.9 | 1.6 | 5.9 | 6.1 |

Table 4. Results for the second working standard (REKLA-1M) in the range of $10^3$ to $10^6$ ions/cc

| Channel | Polarity | Degree of the polynomial |
|---------|----------|-------------------------|
|         |          | 0   | 1   | 2   | 3   |
|         |          | $\delta$ | $v_p$ | $\theta_\Sigma$ | $\delta$ | $v_p$ | $\theta_\Sigma$ | $\delta$ | $v_p$ | $\theta_\Sigma$ |
| 1       | «+»      | 5.3  | 4.2 | 6.8 | 4.0 | 6.0 | 7.2 | 2.7 | 6.1 | 6.7 | 2.0 | 6.5 | 6.8 |
|         | «-»      | 4.9  | 4.0 | 6.3 | 3.5 | 4.3 | 5.5 | 1.4 | 5.5 | 5.7 | 1.4 | 5.7 | 5.9 |
| 2       | «+»      | 4.1  | 4.5 | 6.1 | 3.6 | 5.1 | 6.2 | 3.2 | 6.0 | 6.8 | 2.8 | 6.8 | 7.4 |
|         | «-»      | 4.5  | 5.4 | 7.0 | 4.2 | 5.6 | 7.0 | 1.7 | 5.7 | 5.9 | 1.5 | 6.4 | 6.6 |

It can be seen from the tables that an increase in the degree of the polynomial in the general case reduces the non-excluded residual of the error, but increases the confidence limits of the instability of the metrological characteristics. This is due to the fact that polynomials of high degrees are more sensitive to random outliers of the initial data, which, due to the high random component of the measurement error, can be significant. Note the extremely high values of the non-excluded residual of the error in the lower range at 0 degree of the polynomial (constant correction factor), which reflects a sharp change in the values of the measurement error near the lower limit of the measurement range. The smallest values of the total error are observed at 1 degree of the polynomial in the range $10^3$ - $10^6$ ions/cc and 0 - 2 degrees in the range $10^3$ - $10^6$ ions/cc.

5. Discussion
The proposed method makes it possible to determine the most adequate regression model in cases when the measuring problem is associated with the assessment of the stability of metrological characteristics, and in the
future, with periodic calibration of the investigated SI, this model can be used without additional long-term studies. The method was tested on instruments for measuring the counting concentration of light air ions (LAP). The analysis of the results of measurements of the numeric concentration of light air ions showed that the corrections introduced into the results of measurements by the working standards can be best approximated by two functions in the ranges $10^2 - 10^3$ ions/cc and $10^3 - 10^6$ ions/cc; in which the dependence of the measurement error on concentration has the same form, while at the border of the ranges, the form of this dependence changes sharply. In the lower range, the data can be best approximated by a linear function, in the upper range, by polynomials of powers from 0 to 2 with a logarithmic argument. It is noted that an increase in the degree of the polynomial decreases the non-excluded residual of the error, but increases the confidence limits of the instability of the metrological characteristics during 1-year interval, which occurs due to the high sensitivity of polynomials of high degrees to random outliers of the initial data.

References
[1] R 50.2.004-2000 State system for ensuring uniformity of measurements. Determining the characteristics of mathematical models of dependencies between physical quantities when solving measurement problems. Main provisions (in Rus.)
[2] Blinov A P 1987 Construction of calibration curves of measuring instruments with the method of maximum compactness Measurement Techniques 7 (in Rus.)
[3] RMG 74-2004 State system for ensuring the uniformity of measurements. Methods for determining the intervals of verification and calibration of measuring instruments (in Rus.)
[4] Zubkov P N 2019 Assessment of the stability of the metrological characteristics of measuring instruments during calibration Metrology in the 21st cent. (Abstracts of the VI sci. and tech. conf. of young scientists, graduate students and specialists, VNIIFTRI) pp 29-31 (in Rus.)