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SO_2 in Atmosphere Predicted with Improved Error GM (1,1) Model-Based on Optimization of Initial Condition in Chongqing, China

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To increase the prediction precision of GM (1,1) model, optimization of the initial condition and error GM (1,1) model was integrated for the improvement of original GM (1,1) model. The results of numerical example indicated that the original GM (1,1) model and the improved GM (1,1) model could mostly indicate the average change tendency of reported value and the error GM (1,1) model and the improved error GM (1,1) model both tended to the actual numerical fluctuation. There were significant correlations among predicted value from four GM (1,1) models and reported value and the correlation was 0.953, 0.959, 0.980 and 0.992, respectively. Taking into account the results of correlation analyses, 0.040 to 0.041 mg/L was considered to be the most reasonable predicted concentration range to SO_2 in atmosphere environment of Chongqing, China in 2011. Although the new modified model could improve the prediction accuracy of GM (1,1) model, which was recommended for a small amount of information modeling and prediction, only limited numerical example could be predicted, mainly due to residual error increased in the model.

Key Words: GM (1,1) model, Optimization, Initial condition, Residual error.

INTRODUCTION

Grey systems theory was proposed in 1982[1,2] and became a new discipline researched and used in a variety of fields such as natural science, social science and engineering science, *etc*. The main objects of grey systems theory were small sample or poor information with partial known and partial unknown, which was existed in more system with the development of science and technology. Seeking for rules and characteristics of these uncertain systems became great challenges for further development in associated fields. However, solutions to these problems could be provided by some approaches in grey systems theory.

GM (1,1) model is one of important models in grey systems theory, which could be used to elaborate or analyze events that had not yet been expressed with general functions, but elaborated *via* conception was not clear for the time being. From the procedure of construction, GM (1,1) model is neither a differential equation nor a difference equation, whose characteristic were both differential equation and difference equation. There were some inevitable errors in practical application.

Various reports in the literature indicated many ways to increase prediction accuracy upon improvements of GM (1, 1) model mainly in three aspects, which were improvements of grey derivative, improvements of background value and improvements of the initial condition[3]. Mu[4,5] presented a method to optimize the whitened values of grey derivative and constructs an unbiased GM (1,1) model and proved that the new model had the characteristic of law of whitened exponent. Xie and Liu[6] proposed discretely grey prediction models and corresponding parameter optimization methods and illustrated three classes of grey prediction models such as the starting-point fixed discrete grey model, the middle-point fixed discrete grey model and the ending-point fixed discrete grey model. Mao and Chirwa[7] utilized a modified GM (1,1) model based on background value to predict vehicle fatality risk and obtain a better prediction performance. Liu and Lin[8] presented a method to improve the prediction precision by optimization of the coefficient of exponential function. In addition to these three classes of improvements on GM (1,1) model, Hsu and Wang[9] presented a grey model improved by the Bayesian analysis to predict output of integrated circuit industry.

However, there still existed some space to improve prediction precision of GM (1,1) model. Wang *et al*.[3] pointed that prediction precision of GM (1,1) model could be improved by optimization of the initial condition and the result of a numerical example indicated that the modified GM (1,1) model could obtain a better prediction performance than that from the original GM (1,1) model. Huang *et al.*,[10] proposed an improved error GM (1,1) model to predict cultivated land in Yiyang, based on gray error GM (1,1) model and the results showed that the improved error GM (1,1) model had high prediction precision and better simulation results.

Optimization of the initial condition and error GM (1,1) model was integrated for the improvement of original GM (1,1) model in this paper. The new improved error GM (1,1) model was illustrated through a numerical example, which was the prediction of atmospheric environment quality in Chongqing, China, according to environmental quality bulletins. Whether the proposed methods were helpful for the improvement of original model was also suggested in this paper.

Methods

Original GM (1,1) model:

Assume that

$$X^{(0)} = \left(x^{(0)}(1), x^{(0)}(2), \ldots\ldots, x^{(0)}(n)\right)$$

was a non-negative sequence of raw data and then the AGO of $X^{(0)}$ was denoted as following:

$$X^{(1)} = \left(x^{(1)}(1), x^{(1)}(2), \ldots\ldots, x^{(1)}(n)\right), \text{ where}$$

$$x^{(1)}(k) = \sum_{i=1}^{k} x^{(0)}(i), k = 1,2,\ldots n$$

was obtained from applying the first-order accumulative generation operator on sequence $X^{(0)}$ and then the average of $X^{(1)}$ was as following:

$$Z^{(1)} = (z^{(1)}(2), z^{(1)}(2) z^{(1)}(2)) \text{ where}$$

$$z^{(1)}(k) = \frac{1}{2}(x^{(1)}(k) + x^{(1)}(k-1)), k = 2,3,\ldots\ldots n$$

was a new sequence with the application of the generated mean value of consecutive neighbors operator on $X^{(1)}$, then the following equation,

$$x^{(0)}(k) + az^{(1)}(k) = b$$

was a grey differential equation, also called GM(1,1) model. The restored values of raw data were given below.

$$\hat{x}^{(1)}(k+1) = (x^{(1)} - \frac{b}{a})e^{-ak} + \frac{b}{a}, k = 1,2,\ldots\ldots, n. \quad (1)$$

$$\hat{x}^{(0)}(k+1) = \hat{x}^{(1)}(k+1) - \hat{x}^{(1)}(k) = (1-e^{a})$$
$$(x^{(0)}(1) - \frac{b}{a})e^{-ak}, k = 1,2,\ldots\ldots., n \quad (2)$$

GM (1,1) model with optimization of the initial condition:

To improve prediction precision of GM (1,1) model, Wang *et al.*[3] changed the expression of the above whitened equation:

$$bx^{(1)}(1) = \beta ce^{-a} + \beta^{b}/_{a}$$
$$(1-\beta)x^{(1)}(n) = (1-\beta)ce^{-an} + (1-\beta)^{b}/_{a}$$

where, c was a constant and was an another parameter; where $\beta \in [0,1]$; a and b were parameters derived from the least square estimation method.

$$c = \frac{\beta x^{(1)}(1) + (1-\beta)x^{(1)}(n) - b/a}{\beta e^{-a} + (1-\beta)e^{-an}} \quad (3)$$

Wang *et al.* also constructed a function expressed as following:

$$f(c) = \sum_{k=1}^{n}(\hat{x}^{(1)}(k) - x^{(1)}(k))^2, \text{ let } \frac{df(c)}{dc} = 0, \text{ then}$$

$$\beta = \frac{(x^{(1)}(n) - b/a)\sum_{k=1}^{n} e^{-2ak} - e^{-an}\sum_{k=1}^{n}\left[(x^{(1)}(k) - b/a)e^{-ak}\right]}{(e^{-a} - e^{-an})\sum_{k=1}^{n}\left[(x^{(1)}(k) - b/a)e^{-ak}\right] + (x^{(1)}(n) - x^{(1)}(0))\sum_{k=1}^{n} e^{-2ak}}$$

The optimized time response function was obtained as following,

$$\hat{x}^{(1)}(t) = [\beta x^{(1)}(1) + (1-\beta)x^{(1)}(n) - b/a][\beta e^{-a} + (1-\beta)e^{-an}]e^{-at} + b/a$$
$$= (1-e^{-a})[\beta x^{(1)}(1) + (1-\beta)x^{(1)}(n) - b/a][\beta e^{-a} + (1-\beta)e^{-an}]^{-1}e^{-at} \quad (4)$$

$$\hat{x}^{(0)}(t) = \hat{x}^{(1)}(t) - \hat{x}^{(1)}(t-1)$$

Improved error GM (1,1) model:

$$\varepsilon^{(0)} = (\varepsilon^{(0)}(t_1), \varepsilon^{(0)}(t_2), \ldots\ldots, \varepsilon^{(0)}(t_n))$$

$$\varepsilon^{(0)}(t) = \left|x^{(0)}(t) - \hat{x}^{(0)}(t)\right|$$

was a non-negative sequence of residual error and then the AGO of was denoted as following,

$$\varepsilon^{(1)} = (\varepsilon^{(1)}(t_1), \varepsilon^{(1)}(t_2), \ldots\ldots, \varepsilon^{(1)}(t_n)), \text{ where}$$

$$\varepsilon^{(1)}(t_k) = \sum_{i=1}^{k}(\varepsilon^{(1)}(t_1), k = 1,2,\ldots n$$

was obtained from applying the first-order accumulative generation operator on sequence $\varepsilon^{(0)}$ and then the average of $\varepsilon^{(1)}$ was as following:

$$Z_{\varepsilon}^{(1)}(t_k) = 0.5(\varepsilon^{(1)}(t_k) + \varepsilon^{(1)}(t_{k-1}))$$

$$Z_{\varepsilon}^{(1)} = (Z_{\varepsilon}^{(1)}(t_2), (Z_{\varepsilon}^{(1)}(t_3), \ldots (Z_{\varepsilon}^{(1)}(t_n))$$

was a new sequence with the application of the generated mean value of consecutive neighbors operator on and the restored error value of raw data was given below:

$$\varepsilon^{(0)}(t_k) + az_{\varepsilon}^{(1)}(t_k) = b$$

$$\varepsilon^{(0)}(t_k) = \frac{b - a\varepsilon^{(1)}(t_{k-1})}{1 + 0.5a}$$

From GM (1,1) model with optimization of the initial condition and error GM (1,1) model, the response function was obtained as following:

$$\hat{x}'^{(0)}(t_k) = \hat{x}^{(0)}(t_k) + \varepsilon^{(0)}(t_k)$$
$$= (1-e^{-a})[\beta x^{(1)}(1) + (1-\beta)x^{(1)}(n) - b/a]$$
$$[\beta e^{-a} + (1-\beta)e^{-an}]e^{-dk} + \frac{b - a\varepsilon^{(1)}(t_{k-1})}{1 + 0.5a} \quad (5)$$

Hence, the new modified error GM (1,1) model was an extension of the original error GM (1,1) and the improved GM (1,1) proposed by Wang *et al.*[3].

Example applications: The new improved error GM (1,1) model was illustrated through numerical example. To compare with prediction performances among the original GM (1,1) model, error GM (1,1) model, improved GM (1,1) model and improved error GM (1,1) model, monitoring data of atmosphere environment of Chongqing, China was utilized to construct these four GM (1,1) models, respectively.

TABLE-1
CONCENTRATION OF SO_2 IN ATMOSPHERE ENVIRONMENT OF CHONGQING, CHINA (unit mg/L)

Year	1998	1999	2000	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010
SO_2	0.183	0.171	0.156	0.108	0.091	0.115	0.113	0.073	0.074	0.065	0.063	0.053	0.048

According to the environmental quality bulletins, the monitoring data of SO_2 from 1998 to 2010 was shown in Table-1. Then the non-negative sequence of raw data was:
$X^{(0)} = (x^{(0)}(1), x^{(0)}(2), ..., x^{(0)}(n)) = (0.183, 0.171, 0.156, 0.108, 0.091, 0.115, 0.113, 0.073, 0.074, 0.065, 0.063, 0.053, 0.048)$.

Because the raw data was unqualified, the original series needed square root transformation. First, the parameters were estimated and the original GM (1,1) model was constructed as following: a = 0.0550, b = 0.4344.

$$\hat{x}^{(1)}(k+1) = -7.4753e^{-0.0550k} + 7.9031$$

Second, the parameters were derived and the improved GM (1,1) model was constructed as following: a = 0.0550, b = 0.4344.

$$\hat{x}^{(1)}(k+1) = -7.8977e^{-0.0550k} + 7.9031$$

was the value of square root transformation and the predicted value of those models should be performed on square data.

Third, the error GM (1,1) model and improved error GM (1,1) were constructed as following:

$$\hat{x}'^{(1)}(k+1) = -7.8977e^{-0.0550k} + 0.0003\varepsilon^{(1)}(t_{k-1}) + 7.9369$$

$$\hat{x}'^{(1)}(k+1) = -7.4753e^{-0.0550k} + 0.0001\varepsilon^{(1)}(t_{k-1}) + 7.9210$$

The predicted value of all four models was shown in Table -2.

TABLE-2
PREDICTED VALUE OF ALL FOUR MODELS (unit: mg/L)

Year	Reported value	Predicted value of GM (1,1) model	Predicted value of improved GM (1,1) model	Predicted value of error GM (1,1) model	Predicted value of improved error GM (1,1) model
1998	0.183	0.183	0.183	0.183	0.183
1999	0.171	0.143	0.160	0.143	0.160
2000	0.156	0.128	0.143	0.150	0.167
2001	0.108	0.115	0.128	0.105	0.109
2002	0.091	0.103	0.115	0.094	0.099
2003	0.115	0.092	0.103	0.100	0.117
2004	0.113	0.083	0.092	0.090	0.103
2005	0.073	0.074	0.083	0.068	0.074
2006	0.074	0.066	0.074	0.071	0.068
2007	0.065	0.059	0.066	0.064	0.062
2008	0.063	0.053	0.059	0.057	0.062
2009	0.053	0.048	0.053	0.050	0.052
2010	0.048	0.043	0.048	0.045	0.047
2011	-	0.038	0.043	0.040	0.041

Fig. 1 showed the prediction performance of the original GM (1,1) model and the improved GM (1,1) model. Both of two predictions could mostly indicate the average change tendency of reported value, but there still were a few differences among predicted value of two models and reported value, especially when reported value changed a lot. The predicted trends of two models were relatively stable, but could not reflect the actual numerical fluctuation. However, prediction performance from improved GM (1,1) model was better than that from original GM (1,1) model, because the predicted value of the former predictive value was better than the latter prediction to response average changes of reported value.

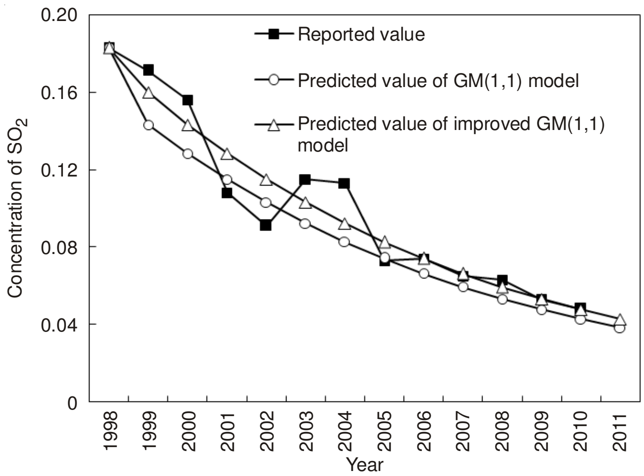

Fig. 1. Predicted value of original and improved

The changes of prediction from error GM (1,1) model and the improved error GM (1,1) model were shown in Fig. 2. Both of two predictions tended to the actual numerical fluctuation. It could be seen from Fig. 2 that the prediction performance from improved error GM (1,1) model was better than that from error GM (1,1) model. Although the predicted trend of error GM (1,1) was similar to reported value, all predicted value was were lower than reported values, which proved that there was still space for improvement in error GM (1,1) model. On the other hand, prediction performance of the improved error GM (1,1) model was almost same to the reported value. It could be shown the improved error GM (1,1) model with optimization of the initial condition was helpful to increase prediction precision of GM (1,1) model.

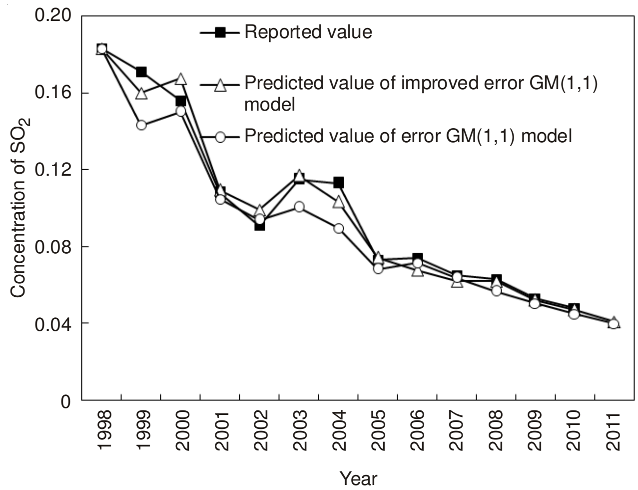

Fig. 2. Predicted value of original and improved

In order to investigate the associated degree between the predicted value and reported value, correlation analyses were proposed with SPSS 15.0. The results were shown in Table-3.

TABLE-3
CORRELATIONS AMONG PREDICTED VALUE FROM FOUR GM (1,1) MODELS AND REPORTED VALUE (N = 13)

	Predicted value of GM (1,1) model	Predicted value of improved GM (1,1) model	Predicted value of error GM (1,1) model	Predicted value of improved error GM (1,1) model
Reported value	0.953**	0.959**	0.980**	0.992**

**Correlation was significant at the 0.01 level

From Table-3, it could be concluded that there were significant correlations among predicted value from four GM (1, 1) models and reported value and the correlation between predicted value of improved error GM (1,1) model and reported value was the highest, while the correlation between predicted value of GM (1,1) model and reported value was the lowest. The predicted concentration of SO_2 in 2011 from all four models was presented in Table-2, which was 0.038 mg/L, 0.043 mg/L, 0.040 mg/L and 0.041 mg/L, respectively. Taking into account the results of correlation analyses, 0.040 mg/L to 0.041 mg/L was considered to be the most reasonable predicted concentration range to SO_2 in atmosphere environment of Chongqing, China in 2011. The above reasonable concentration range could meet the class-II demand of air quality standards of China, which was ≤ 0.6 mg/L.

Conclusion

Four GM (1,1) models was indicated in this paper, which was original GM (1,1) model, error GM (1,1) model, improved GM (1,1) model and improved error GM (1,1) model with optimization of the initial condition, respectively. The results of numerical example indicated that the original GM (1,1) model and the improved GM (1,1) model could mostly indicate the average change tendency of reported value and the error GM (1,1) model and the improved error GM (1,1) model, which was the new modified model, both tended to the actual numerical fluctuation. The new modified model was an extension of the original GM (1,1) model and the error GM (1,1) model and it could improve the prediction precision of GM (1,1) model, which was recommended for a small amount of information modeling and prediction. When using the new defined model, only limited numerical example could be predicted, mainly due to residual error increased in the model. With the results of prediction of models and correlation analyses, 0.040 mg/L to 0.041 mg/L was considered to be the most reasonable predicted concentration range to SO_2 in atmosphere environment of Chongqing, China in 2011.

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