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Forecasting of dissolved oxygen in the Guanting reservoir using an optimized NGBM (1,1) model

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A B S T R A C T

An optimized nonlinear grey Bernoulli model was proposed by using a particle swarm optimization algorithm to solve the parameter optimization problem. In addition, each item in the first-order accumulated generating sequence was set in turn as an initial condition to determine which alternative would yield the highest forecasting accuracy. To test the forecasting performance, the optimized models with different initial conditions were then used to simulate dissolved oxygen concentrations in the Guanting reservoir inlet and outlet (China). The empirical results show that the optimized model can remarkably improve forecasting accuracy, and the particle swarm optimization technique is a good tool to solve parameter optimization problems. What’s more, the optimized model with an initial condition that performs well in in-sample simulation may not do as well as in out-of-sample forecasting.

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Keywords:
Water quality forecasting
Dissolved oxygen
Nonlinear grey Bernoulli model
Particle swarm optimization
Initial condition

Introduction

Surface water quality is a hot environmental issue because of its importance in human health and ecological systems (Voysslov et al., 2012; Chen et al., 2014; Tanaka et al., 2013). Dissolved oxygen (DO) is one of the most important water quality parameters, and forecasting DO in surface water is a big concern for water resource management. Many models have been developed to forecast DO in water bodies (Heddam, 2014; Matos and de Sousa, 1996; Liu et al., 2014; Singh et al., 2014). Neural network, a widely used method in DO forecasting, can obtain high simulation and forecasting accuracy (Wen et al., 2013; Areerachakul et al., 2013; Ranković et al., 2010; Heddam, 2014). However, the application of the neural network method typically requires large amounts of input data. Grey system theory, proposed by Deng (1982), was specially designed to study systems with incomplete or uncertain information. Limited data are available to estimate the behavior of an unknown system, making grey models useful for systems with scarce information. GM (1,1) constructed by exponential functions is one of the most widely used grey models (Lee et al., 2007; Jiang, 1995). GM (1,1) only requires four data values to forecast the parameters of a system with a reasonable degree of accuracy.

Many methods have been used to improve the accuracy of the traditional grey forecasting model GM (1,1) to some extent (Li et al., 2011; Hsu and Chen, 2003).

In this article, the nonlinear grey Bernoulli model (NGBM (1,1)) proposed by Chen (2008) and Chen et al. (2008) is tested for its effectiveness. NGBM (1,1) is a simple modification of GM (1,1) using the Bernoulli differential equation. Unlike GM (1,1) and the grey Verhulst model (GVM), relying on a constant number such as 0 and 2, NGBM (1,1) possesses a power exponent r to determine the shape of model’s curve. When r is equal to 0, NGBM (1,1) degenerates to GM (1,1), while when r is equivalent to 2, NGBM (1,1) possesses a power exponent r to determine the shape of model’s curve. When r is equal to 0, NGBM (1,1) degenerates to GM (1,1), while when r is equivalent to 2, NGBM (1,1) becomes GVM. This demonstrates that NGBM (1,1) has greater flexibility than GM (1,1) and GVM through adjustment of the parameter r. Besides the parameter r, the production coefficient of the background value p is another parameter that needs to be improved. The value p in grey models is determined by the developing coefficient a (Luo et al., 2003; Zhou et al., 2009). Thus, it is inaccurate to customarily set the value p to 0.5. The values r and p in NGBM (1,1) have been successfully improved to enhance the modeling precision (Chen, 2008; Hsu, 2010; Pao et al., 2012; Zhou et al., 2009; Chen et al., 2010; Wang et al., 2011; Zhang et al., 2014). First, a simple computer program (Chen, 2008), a
Step 2: Perform the accumulated generating operation on

Step 3: The grey differential equation of NGBM (1,1) is defined

values and the original accumulating generation values, respec-
tively, and between the simulat ed accumulating generation
square error between the simulated values and the observed
values.

Wang et al. (2010) used the weighted
generating sequence, and the last item was taken to be the initial
condition (Dang et al., 2005). Wang et al. (2010) were utilized to simultaneously determine the
values r and p, and the optimized model further improved the
forecasting precision. In this study, according to its ability in
optimizing difficult multidimensional discontinuous problems,
PSO was chosen to solve the parameter optimization problem.

Most improvements of NGBM (1,1) have focused on the values
r and p. However, studies on both the initial condition and the
two adjustable parameters in the NGBM (1,1) model are scarce
(Wang, 2013a). The initial condition in grey models is also an
important factor affecting the simulation and forecasting preci-
sion. According to grey system theory, the model should give
priority to new information. Thus, the initial condition should
not be limited to the first item in the first-order accumulated
generating sequence, and the last item was taken to be the initial
condition (Dang et al., 2005). Wang et al. (2010) used the weighted
sum of the first item and the last item as the initial condition.
Xu and Leng (1999) and Liu et al. (2003) minimized the sum of the
square error between the simulated values and the observed
values, and between the simulated accumulating generation
values and the original accumulating generation values, respec-
tively. In this study, different initial conditions (Zhang et al., 2002)
combined with the optimized model were tested to research the
effectiveness of the NGBM (1,1) model.

1. Methodology

1.1. Nonlinear grey Bernoulli model

The procedures of NGBM (1,1) can be concluded as follows.

Step 1: Let \( X^{(0)} \) be a non-negative data sequence

\[
X^{(0)} = [x^{(0)}(1), x^{(0)}(2), x^{(0)}(3), \ldots, x^{(0)}(n)],
\]

where, \( x^{(0)}(k) \) is the \( k \)th value of \( X^{(0)} \), \( k = 1, 2, \ldots, n \).

Step 2: Perform the accumulated generating operation on \( X^{(0)} \) as:

\[
X^{(1)} = [x^{(1)}(1), x^{(1)}(2), x^{(1)}(3), \ldots, x^{(1)}(n)],
\]

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

Step 3: The grey differential equation of NGBM (1,1) is defined as:

\[
x^{(0)}(k) + ax^{(1)}(k) = b \left[ x^{(1)}(k) \right]^r,
\]

and its whitening differential equation is as follows,

\[
\frac{dx^{(1)}}{dt} + ax^{(1)} = b \left[ x^{(1)} \right]^r,
\]

where, \( x^{(0)}(k) = px^{(0)}(k) + (1-p)x^{(0)}(k-1) \), \( k = 2, 3, 4, \ldots, n \); \( p \) is called the production coefficient of the background
value with a close interval \([0,1]\); \( r \) is an adjustable parameter, belonging to any real number excluding \( r = 1 \).

Step 4: In order to estimate the parameters \( a \) and \( b \), using the
least squares method, Eq. (3) is approximated as:

\[
[a, b]^T = [B^T B]^{-1} B^T y,
\]

where,

\[
B = \begin{bmatrix}
-Z^{(1)}(2) & Z^{(1)}(2) \\
-Z^{(1)}(3) & Z^{(1)}(3) \\
-Z^{(1)}(4) & Z^{(1)}(4) \\
\vdots & \vdots \\
-Z^{(1)}(n) & Z^{(1)}(n)
\end{bmatrix}, \quad Y = \begin{bmatrix}
x^{(0)}(2) \\
x^{(0)}(3) \\
x^{(0)}(4) \\
\vdots \\
x^{(0)}(n)
\end{bmatrix}.
\]

Step 5: Set the initial condition \( x^{(1)}(1) = x^{(1)}(1) \), and the
solution of Eq. (4) can be expressed as:

\[
x^{(1)}(k) = \left( x^{(1)}(1)^{1-r} - \frac{b}{a} \right) e^{\left( \frac{b}{a} \right) (k-1)} + \frac{b}{a} \left( \frac{x^{(0)}(1)}{a} \right)^{1-r}, \quad r \neq 1, k = 1, 2, \ldots.
\]

Let the initial condition \( x^{(1)}(m) = x^{(1)}(m) \) (\( m = 2, 3, \ldots, n \)), and the particular solution of Eq. (4) is:

\[
x^{(1)}(k) = \left( x^{(1)}(m)^{1-r} - \frac{b}{a} \right) e^{\left( \frac{b}{a} \right) (k-m)} + \frac{b}{a} \left( \frac{x^{(0)}(m)}{a} \right)^{1-r}, \quad r \neq 1, k = 1, 2, \ldots.
\]

Step 6: The inverse accumulated generating operation is
performed on \( x^{(1)}(k) \), and the forecasted value of \( x^{(0)}(k) \) can be estimated as:

\[
x^{(0)}(1) = x^{(0)}(1),
\]

\[
x^{(0)}(k) = x^{(1)}(k) - x^{(1)}(k-1), \quad k = 2, 3, \ldots.
\]

The adjustable parameters \( r \) and \( p \) need to be
determined by the original data sequence. Therefore,
how to acquire the appropriate values of \( r \) and \( p \) is an
important issue in NGBM (1,1) applications.

1.2. The PSO algorithm

The PSO algorithm was designed and introduced by Kennedy
and Eberhart (1995), and was inspired by the motion of a
school of birds looking for food. The main idea of PSO is to
search for the optimal solution by cooperation and informa-
tion sharing. In PSO language, the population is referred to as
a swarm and each individual in the swarm is called a particle.
Particles are initialized with a randomized velocity and
position. The optimal or approximately optimal solution can
be found from iteration to iteration. Each particle is iteratively
updated by its own best fitness value and the best fitness
value of the entire swarm so far.

A particle represents a point in D-dimension space, and its
status can be characterized by its position and velocity. The
position for the \( i \)th particle at the \( k \)th iteration is described as
   \( X_i = (x_{i1}, x_{i2}, \ldots, x_{id}) \).
The velocity for the \( i \)th particle at the \( k \)th iteration can be denoted as
   \( V_i = (v_{i1}, v_{i2}, \ldots, v_{id}). \) The fitness value of each particle is decided by the objective function of the
Step 6: If the stopping iteration condition is not met, loop to

\[ v_{id}^{k+1} = w^k v_{id}^k + c_1 r_1 (p_{id}^k - x_{id}^k) + c_2 r_2 (p_{id}^* - x_{id}^k), \]  

\[ x_{id}^{k+1} = x_{id}^k + v_{id}^{k+1}, \quad d = 1, 2, \ldots, D. \]  

where, \( w^k \) is the inertia weight at the \( k \)th iteration. Shi and Eberhart (1998a) introduced an inertia weight, and found that a dynamic \( w^k \) value can acquire better optimal parameters. Linearly decreasing weight was used in this study (Shi and Eberhart, 1998b; Chen and Zhao, 2009). The capability of global search increases with a large inertia weight and a small inertia weight facilitates a local search. In Eq. (11), \( k \) is the current generation and max is the maximum generation in each experiment, and initial inertia weight \( w_{max} \) is 0.9, final inertia weight \( w_{min} \) is 0.4. In Eq. (10), \( c_1 \) and \( c_2 \) are acceleration factors to control the maximum step size, \( r_1 \) and \( r_2 \) are random numbers in the interval between zero and one.

The procedure of the PSO algorithm is summarized as follows:

Step 1: Initialize a population of particles, including random positions and velocities in \( D \) dimensions.

Step 2: Estimate the fitness value of each particle.

Step 3: For each particle, compare the fitness value with its previous best value. If the current fitness value is better than its previous best value, the current value is updated to be previous best value.

Step 4: For each particle, compare its fitness value with the population’s previous best value. If the current fitness value is better than the overall previous best value, the current value is updated to the current particle’s array index and value.

Step 5: Update the velocity and position of each particle according to Eqs. (10)-(12).

Step 6: If the stopping iteration condition is met, loop to Step 2. The stopping iteration is usually referred to a maximum number of iterations or a sufficiently good fitness value.

The PSO algorithm was carried out by MATLAB 8.0 to find the optimal values of \( r \) and \( p \). The PSO parameter values were set as: maximum number of iterations is 300; population size is 40; \( c_1 \) and \( c_2 \) are both 2; and initial inertia weight and final inertia weight are 0.9 and 0.4, respectively.

1.3. Optimal parameter estimation

The mean absolute percentage error (MAPE) is a way to evaluate the simulation and forecasting performance. The lowest MAPE means highest accuracy and good consistency between forecasted values and actual values, which is the purpose for optimizing parameters in the NGBM (1,1) model.

The parameters \( r \) and \( p \) are optimized with objective function MAPE, based on the initial condition varying from \( x^{(1)}(1) \) to \( x^{(6)}(n) \).

When \( x^{(1)}(1) \) is the initial condition, the problem of optimal parameter estimation can be formulated as below

\[
\text{Min MAPE} = \left( \frac{1}{n-1} \sum_{n=2}^{n} \left| \frac{x^{(k)}(k) - \hat{x}^{(k)}(k)}{x^{(k)}(k)} \right| \right) \times 100\%. \tag{13}
\]

When \( x^{(m)}(m) \) \((m = 2, 3, \ldots, n)\) is taken as the initial condition, the objective function is shown as:

\[
\text{Min MAPE} = \left( \frac{1}{n-1} \sum_{n=2}^{n} \left| \frac{x^{(k)}(k) - \hat{x}^{(k)}(k)}{x^{(k)}(k)} \right| \right) \times 100\%. \tag{14}
\]

2. Validation of the optimized NGBM (1,1) model

In this section, two numerical examples, a fluctuating data sequence and a monotonically increasing data sequence, were utilized to demonstrate the advantages of the optimized NGBM (1,1) model.

2.1. A fluctuating data sequence

A fluctuating data sequence \( X^{(0)} = \{1, 2, 3, 4, 5, 6\} \) (Data sequence A) (Wang, 2013b) was chosen to be an example to indicate the improvement in forecasting accuracy of the optimized NGBM (1,1) models with different initial conditions. Simulation results are shown in Table 1.

Table 1 reveals that the optimized NGBM (1,1) using \( x^{(3)}(2) \) as the initial condition has a higher simulation accuracy than those with the other initial conditions. The MAPE of the optimized NGBM (1,1) model with \( x^{(3)}(2) \) as the initial condition increased from 6.1205% to 4.0105%. Overall, the difference of MAPEs among the optimized NGBM (1,1) models with different initial conditions is small, and the fitting effect with \( x^{(3)}(2) \) as the initial condition on the same data sequence is better than the optimized models with the other initial conditions.

2.2. A monotonically increasing data sequence

Like the fluctuating data sequence, a monotonically increasing data sequence (Data sequence B) (Chen, 1990; Yu, 1991) was used to assess the simulation accuracy of the optimized NGBM (1,1) models with different initial conditions. The simulation results of the optimized NGBM (1,1) models using different initial conditions are shown in Table 2. As can be

| Table 1 – Simulation results of data sequence A. |
|-----------------|-----------------|-----------------|
| Initial condition | \( p \) | \( r \) | MAPE (%) |
| \( x^{(1)}(1) \)  | 0.4407          | 1.6992          | 6.1205    |
| \( x^{(2)}(2) \)  | 0.4602          | 1.3535          | 4.0105    |
| \( x^{(3)}(3) \)  | 0.4451          | 1.4527          | 4.0461    |
| \( x^{(4)}(4) \)  | 0.5029          | 1.3878          | 5.2296    |
| \( x^{(5)}(5) \)  | 0.5029          | 1.3878          | 5.2296    |

\( x^{(6)}(6) \)  | 0.5029          | 1.3878          | 5.2296 |
seen in Table 2, the optimized NGBM (1,1) model with \( x^{(1)}(6) \) as the initial condition obtains the best fitting effect with the minimum MAPE (24.121%).

To show the superiority of the optimized model in handling a data sequence having nonlinear variations, the MAPEs of GM (1,1), GVM and NGBM (1,1) using \( x^{(1)}(1) \) as the initial condition for Data sequence A and Data sequence B are compared in Table 3.

From Table 3, the MAPEs for Data sequence A of GVM and NGBM (1,1) are 15.056% and 6.1205%, respectively. GM (1,1) returns no value because the developing coefficient \( a \) is calculated as 0. The MAPEs for the Data sequence B of the three grey models are 289.48%, 114.52%, and 24.22%, respectively. In general, the optimized NGBM (1,1) achieves the highest simulation precision among the three grey models both for Data sequence A and Data sequence B. The performance comparisons show that the optimized NGBM (1,1) is effective and suitable in coping with data sequences having nonlinear variations.

3. Forecasting DO in the Guanting reservoir inlet and outlet

3.1. Materials

Guanting reservoir is located at the upper reaches of the Yongding River in the northwest of Beijing. It was the first large reservoir built after the foundation of the People's Republic of China, with a catchment area of 43,402 km\(^2\) and storage capacity of 4.16 billion m\(^3\) (Yang and Xu, 2009). The Sangganhe River, Yanghe River, and Weishuihe River flow into the Guanting reservoir. Guanting reservoir once served as Beijing’s second largest source of water. However, Guanting reservoir has not providing drinking water for Beijing since 1997, because it was polluted by industrial wastewater and domestic sewage. With the development of society, drinking water consumption is increasing. Therefore, the local government decided to restore the Guanting reservoir to being the second drinking water source.

In this study, DO in the Guanting reservoir inlet (Zhangjia-kou No. 8 bridge monitoring station) and outlet (Beijing Yanhecheng monitoring station) were chosen as the research target. The data for the Guanting reservoir inlet and outlet from Week 34 to Week 43 in 2013 were used for in-sample simulation, while data of Week 44 and Week 45 in 2013 were used for out-of-sample forecasting. The data used in this paper were collected from the Ministry of Environmental Protection of the People's Republic of China.

4. Results and discussion

The PSO algorithm parameter values in this paper were set as mentioned in Section 1.2. Taking \( x^{(1)}(2) \) as the initial condition in the Guanting reservoir inlet and outlet as an example, the evolution of fitness of the optimized NGBM (1,1) model is shown in Fig. 1, respectively. As can be seen in Fig. 1, the fitness value (objective function) converges very fast to a stationary value, demonstrating the high efficiency of the PSO technique to solve the parameter optimization problem.

![Fig. 1 – Evolution of fitness of the optimized NGBM (1,1) with \( x^{(1)}(2) \) for the Guanting reservoir inlet (a) and outlet (b).](image-url)
The simulation and forecasting results achieved by the optimized NGBM (1,1) models with the initial condition varying from \( x^{(1)} \) to \( x^{(n)} \) for the Guanting reservoir inlet and outlet are shown in Tables 4 and 5, respectively. From Table 4, minimum MAPE (3.3732%) for in-sample simulation and optimal parameters estimation \( (p = 0.5771, \quad r = -0.0585) \) are obtained with \( x^{(2)} \) as the initial condition, while the forecasting effect of the optimized model with \( x^{(7)} \) as the initial condition \( (\text{APE for Week 44 is 1.9208%}, \quad \text{APE for Week 45 is 1.7953%}) \) is better than those with the other initial conditions. The highest MAPE (4.4729%) is acquired with \( x^{(5)} \) as the initial condition, and the highest APEs (3.9014%, 8.5195%) are obtained with \( x^{(10)} \) as the initial condition.

From Table 5, the lowest MAPE (3.0309%) for simulation is obtained with \( x^{(2)} \) as the initial condition, while the best forecasting effect is obtained with \( x^{(6)} \) as the initial condition \( (\text{APE for Week 44 is 0.0343%}, \quad \text{APE for Week 45 is 2.378%}) \) is better than those with the other initial conditions. The highest MAPE (4.4729%) is acquired with \( x^{(5)} \) as the initial condition, and the highest APEs (3.6992%, 8.5195%) are obtained with \( x^{(10)} \) as the initial condition.

According to Tables 4 and 5, the optimized NGBM (1,1) models with different initial conditions perform well in simulation and forecasting. However, the forecasting accuracy does not remain consistent with the simulation accuracy. The minimum MAPE (3.3732%) for the simulation of the Guanting reservoir inlet is obtained when \( x^{(2)} \) is set as the initial condition, while the lowest APEs (0.0343%, 2.378%) are gained with \( x^{(7)} \) as the initial condition. In the same way, the outlet simulation results using \( x^{(2)} \) as the initial condition have the highest accuracy, while the optimized model performs best with the minimum APEs (1.9208%, 1.7953%) when \( x^{(6)} \) is set as the initial condition.

The validation and empirical results indicate that using \( x^{(n)} \) as the initial condition is not better than the traditional method \( (x^{(1)} \text{ set as the initial condition}) \) (Zhang et al., 2002; Wang, 2013a).

### 5. Conclusions and future work

NGBM (1,1), a simple modification of GM (1,1) with the Bernoulli differential equation, can be used to forecast small sample time series. The PSO technique of simultaneously optimizing the power index \( r \) and the production coefficient of the background value \( p \) is introduced in the NGBM (1,1) model to improve its simulation and forecasting performance. Moreover, the initial condition is set from \( x^{(1)} \) to \( x^{(n)} \) to obtain the highest simulation and forecasting precision. The optimized NGBM (1,1) models with different initial conditions are employed in the simulation and forecasting DO in the Guanting reservoir inlet and outlet (China).

The validation results of the optimized NGBM (1,1) models with different initial conditions reveal that the optimized model performs the best among the three grey models. The empirical results show that the optimized NGBM (1,1) model has a strong adaptability to the original nonlinear data sequence, and the PSO algorithm is an effective and efficient tool to solve the parameter optimization problem in the NGBM (1,1) model. What’s more, the optimized model with an initial condition that performs well in in-sample simulation may not do as well as in out-of-sample forecasting. Overall, the simulation and forecasting performance is satisfactory.

<table>
<thead>
<tr>
<th>Initial condition</th>
<th>( p )</th>
<th>( r )</th>
<th>MAPE (%)</th>
<th>Week 44 APE (%)</th>
<th>Week 45 APE (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( x^{(1)} )</td>
<td>0.907</td>
<td>-0.0905</td>
<td>3.3675</td>
<td>8.9806</td>
<td>5.1679</td>
</tr>
<tr>
<td>( x^{(2)} )</td>
<td>0.907</td>
<td>-0.0905</td>
<td>3.0309</td>
<td>8.9806</td>
<td>5.1679</td>
</tr>
<tr>
<td>( x^{(3)} )</td>
<td>0.9533</td>
<td>-0.1722</td>
<td>3.1939</td>
<td>9.0909</td>
<td>4.0032</td>
</tr>
<tr>
<td>( x^{(4)} )</td>
<td>0.9744</td>
<td>-0.2132</td>
<td>3.2871</td>
<td>9.1444</td>
<td>3.4382</td>
</tr>
<tr>
<td>( x^{(5)} )</td>
<td>0.9717</td>
<td>-0.2079</td>
<td>3.2747</td>
<td>9.1376</td>
<td>3.51</td>
</tr>
<tr>
<td>( x^{(6)} )</td>
<td>0.0013</td>
<td>-0.0595</td>
<td>3.6992</td>
<td>9.2881</td>
<td>1.9208</td>
</tr>
<tr>
<td>( x^{(7)} )</td>
<td>0.6763</td>
<td>-0.0896</td>
<td>3.1153</td>
<td>9.0697</td>
<td>4.227</td>
</tr>
<tr>
<td>( x^{(8)} )</td>
<td>0.5992</td>
<td>-0.0898</td>
<td>3.3184</td>
<td>8.9392</td>
<td>5.6051</td>
</tr>
<tr>
<td>( x^{(9)} )</td>
<td>1</td>
<td>-0.00901</td>
<td>3.2754</td>
<td>8.9404</td>
<td>5.5924</td>
</tr>
<tr>
<td>( x^{(10)} )</td>
<td>0.5377</td>
<td>-0.0898</td>
<td>3.1697</td>
<td>9.1287</td>
<td>3.604</td>
</tr>
</tbody>
</table>
Considering that grey models are customarily applied to short-term forecasting, the computational complexity is acceptable. Therefore, the different initial conditions can be calculated in the optimized NGBM (1,1) model to achieve the highest simulation and forecasting accuracy.

Using as the initial condition each item in the first-order accumulated generating sequence does increase the computational complexity to some degree, although it is acceptable. In the future, we will try some methods to obtain the weighted sum of $x^{(1)}(t)$ and $x^{(0)}(n)$ as the initial condition to simplify the computational procedure. Meanwhile, in future work the new method and the method in this paper will be compared.

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