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A Data-Driven Iterative Optimization Compensation Method Based on PJIT-PLS for Gold Cyanidation Leaching Process

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ABSTRACT Gold cyanidation leaching process (GCLP) as the central unit operation in hydrometallurgy, which suffers from the problem of the optimal setting point based-model is difficult to reach the optimal working point in actual GCLP due to model error, which leads to lower economic benefit. Meanwhile, the process data contains noise and uncertainty on account of the fluctuation of raw material properties. Therefore, how to take the most of that data to make the production process run in the optimal state of economic benefit under the premise that the quality index meets the production requirements is an urgent problem to be solved. In this paper, a data-driven iterative optimization compensation strategy is proposed to solve aforementioned problems. Firstly, probabilistic principle component analysis (PPCA) method is used to preprocess process data for eliminating the effect of noise and uncertainty; Secondly, two relevant models are established between the operating variable increment and the economic benefit increment, the quality index increment based on just in time (JIT) and partial least squares (PLS) method; Finally, the optimal operating variable increment that maximizes the economic benefit increment can be optimized under the condition of quality index satisfies the production requirements and iterated at the new working point, which is constantly close to the optimal working point to improve the economic benefit. Simulation studies have verified the validity of proposed method.

INDEX TERMS GCLP, data-driven, iterative optimization compensation, PPCA, JIT.

I. INTRODUCTION

With the rapid development of the world economy, high-grade mineral resources are depleted seriously. It is an urgent problem that how to extract non-ferrous metals from low-grade complex mines. Hydrometallurgical process is widely used in the field of non-ferrous metal smelting due to its advantages of low pollution and sustainable. GCLP always plays an important role in hydrometallurgical process as the central operation unit, thus it has been applied successfully in hydrometallurgical plants thanks to simple structure, easy adjustment and low consumption [1]. Residue gold concentration as the key quality index directly impact on the sequent process such as washing, filter press and gold recovered by zinc, thus having a significant effect on the final gold recovery rate (the residue gold concentration is required to be less than 15 in the actual GCLP). Therefore, it is a critical problem how to keep the GCLP running at an optimal economic efficiency state under the premise that the residue gold concentration meet the production requirements.

Establishing GCLP model between the operating variables and the key quality index is the most important basis for implementing indicator prediction and process control [1]. In terms of GCLP modeling, researchers have done some related work [2], [3]. De Andrade et al proposed two lumped

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kinetic models for gold ore cyanidation, which are the kinetic equation of gold dissolution and the cyanide consumption, respectively [2]. Based on kinetic equations for gold ore cyanidation and the mass conservation equations, a steady-state mechanistic model for GCLP is proposed [3]. However, it is difficult to establish an accurate mechanistic model in actual industrial process due to the complex inner mechanism and long process flow. To cope with this problem, data-driven modeling methods are extensively used in industrial plants [4]. They are many kinds of data-driven modeling approaches like multivariate statistical methods such as principle component regression (PCR) [5], independent component regression (ICR) [6], [7], partial least squares (PLS) [8], and nonlinear methods such as kernel PLS [9], kernel PCR [10] and so on. Meanwhile, the machine learning methods have been widely applied in process modeling such as Gaussian process regression (GPR) [11], [12], support vector regression (SVR) [13], artificial neural networks (ANN) [14], [15], their application study has been analyzed in the literature [8], [16]. To solve the kinetic reaction rate expressions are difficult to be obtained accurately in the actual GCLP, Zhang J et al proposed a serial hybrid modeling method that combined the first-principle model (the mass conservation equations in steady-state mechanistic model) and data-driven model (two BP ANN models) [17]. Liu Y et al proposed a state evaluate method for the whole of the gold hydrometallurgical process, using a total projection to latent structures method to evaluate the current production state [18].

However, the process model may degradation owing to the process plants usually undergo different kinds of process characteristic changes like process drifts and equipment aging, change of raw materials etc, which may result in optimal setting point model-based are often not the optimal working point for actual production process, so how to keep GCLP running at the optimal production state become a problem that needs to be solved in process control. Zhang J et al proposed a real time optimization strategy for GCLP based on sufficient conditions for feasibility and optimality to ensure that GCLP runs in an optimal state under the condition of process disturbance and model-parameter uncertainty [1]. Li K et al proposed a data-based compensation method for optimal setting of hydrometallurgical process, which combines the advantages of model-based approach and data-based approach, in the vicinity of the optimal setting point based on model optimization, the data-based local modeling method is used to compensate the operating variables, thereby improving the economic benefit of the production process [19]. However, it does not consider whether the quality index meet the production requirements during iterative compensation process. Meanwhile, the process data contains noise and uncertainty due to the fluctuation of raw material properties.

This paper proposes a data-driven iterative optimization compensation method that under the condition of quality index meet the requirements to solve

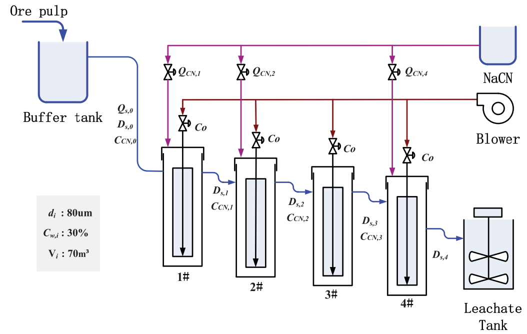

FIGURE 1. The plant flowsheet of four-level GCLP.

aforementioned problem. Specifically, PPCA method is applied to preprocess the data in order to eliminate the effect of noise and uncertainty, and the relevant sample sets that similar to the current optimal setting point based on soft sensor model which was selected from historical database based on JIT, and then two relevant models are established between operating variable increment and the economic benefit increment, the quality index increment based on PLS; the optimal operating variable increment can be optimized by PSO under the condition of quality index satisfy the production requirement and iterated at the new working point, which constantly close to the optimal working point based on the actual GCLP, thus further improved the economic benefit of the production process.

The remainder of this paper is organized as follows: Section 2 gives the brief process description and mechanistic model of GCLP, the main theoretical methods used in this work and the description of optimization setting compensation problem in GCLP. The detailed description of a data-driven iterative optimization compensation method is given in Section 3. Section 4 demonstrates the effectiveness of the proposed method by simulation. Finally, Section 5 presents our conclusions.

II. PRELIMINARIES

A. PROCESS DESCRIPTION

Extracting gold from ores in alkaline cyanide pulp has been the most commonly applied technique in the vast majority hydrometallurgical plants [1]. The plant flowsheet of four-level GCLP is shown in Fig. 1. Ore pulp from tailings is stored in a buffer tank after concentration, pressure filtration, which overflow into the 1# leaching tank continuously and stably. Then, the leachate overflow into the 2#-4# leaching tank and identical reactions occur so as to extract more gold, which is reserved in the leachate tank for the subsequent operations when the GCLP is completed. The use of a blower to introduce compressed air into the leaching tank not only acts as a pneumatic agitation but also provides dissolved oxygen required for the reaction. For the detailed process description of GCLP please refer to [1]- [3], [17] and it will not be covered here.

Recently, related scholars have conducted in-depth research on the reaction mechanism of GCLP [1], [2], [20]. It was confirmed that the main electrochemical reaction occurred as in (1), that is the insoluble gold reacts with sodium cyanide to form soluble $Au(CN)_2^-$, in order to realize the separation of gold and impurities in the ore [2], [20].

$$4Au + 8CN^- + O_2 + 2H_2O \rightarrow 4Au(CN)_2^- + 4OH^- \quad (1)$$

The steady-state mechanistic model for GCLP are composed of mass conservation equations of gold in the solid phase and cyanide in the liquid phase [1], [2], take $i-th$ level as an example, which can be described by (2) and (3), respectively:

$$Q_{s,i}(D_{s,i-1} - D_{s,i}) - r_{Au,i}M_{s,i} = 0 \quad (2)$$

$$Q_{l,i}(C_{CN,i-1} - C_{CN,i}) + Q_{CN,i} - r_{CN,i}M_{l,i} = 0 \quad (3)$$

$r_{Au,i}$,$r_{CN,i}$are the dissolution rate of gold and the rate of consumption of cyanide in the reaction kinetic equation, respectively [2], [3], which are shown in (4) and (5):

$$\begin{aligned} r_{Au,i} &= (1.13 \times 10^{-3} - 4.37 \times 10^{-11}\bar{d}^{2.93}) \\ &\quad \times (D_{s,i} - D_{s\infty}(\bar{d}))^{1.10}C_{CN,i}{}^{0.991}C_{o,i}{}^{0.228} \end{aligned} \quad (4)$$

$$r_{CN,i} = \frac{1.69 \times 10^{-8}}{\bar{d}^{0.547} - 6.40}C_{CN,i}{}^{2.91} \quad (5)$$

Among them, the grade of gold remaining in the ore after GCLP is under ideal condition, which is a function of the average particle size $\bar{d}$ of the ore [2]:

$$D_{s\infty}(\bar{d}) = 0.357(1 - 1.49e^{-1.76\times10^{-2}\bar{d}}) \quad (6)$$

Finally, the values of operation conditions and process variables of the GCLP shown in Table 1 and Table 2. The input of steady-state mechanistic model for the GCLP is $x = [Q_{CN,1}, Q_{CN,2}, Q_{CN,4}]$, the output is $D_{s,4}$, which can be expressed by y, the relationship of which can be described by:

$$y = f_m(x) \quad (7)$$

B. THE MAIN THEORETICAL METHODS

1) PROBABILISTIC PRINCIPLE COMPONENT ANALYSIS (PPCA)

PPCA is an extension of deterministic principle component analysis (PCA), the purpose of which is to effectively tackle data noise and uncertainty by define PCA as a probability model [21]. In PPCA, the observed variables can be generated from latent variables by the following factor generation model [21], [22], [24]:

$$x = wz + u + \varepsilon \quad (8)$$

where $x = \{x_1, x_2, ..., x_n\} \in r^{m\times n}$ is the observed variables. n and m represent the number of samples and variables respectively. $w \in r^{m\times q}$ is the loading matrix, q represents the number of principal components $q < m$. $z \in r^{q\times n}$ is the latent variables, u is the bias term or mean of the observed

TABLE 1. The values of process variables of the GCLP.

Symbol	Variable	Unit
$D_{s,0}$	initial gold concentration in the ore	mg/kg
$D_{s,i}$	gold concentration in the ore	mg/kg
$D_{s\infty}$	residual gold concentration in the ore	mg/kg
$C_{CN,i-1}$	initial cyanide concentration in the liquid	mg/kg
$C_{CN,i}$	cyanide concentration in the liquid	mg/kg
$C_{o,i}$	oxygen concentration in the liquid	mg/kg
$\bar{d}$	average size of the ore particles	μm
$M_{s,i}$	ore hold-up	kg
$M_{l,i}$	liquid hold-up	kg
$Q_{s,i}$	ore flow rate	kg/h
$Q_{l,i}$	liquid flow rate	kg/h
$Q_{CN,i}$	cyanide flow rate added	mg/h
$r_{Au,i}$	dissolution rate of gold	mg/(kgh)
$r_{Cu,i}$	consumption rate of cyanide	mg/(kgh)
N	leaching levels	-
i	$i-th$ leaching tank	-

TABLE 2. The values of operation conditions of the GCLP.

$Q_{s,i}$	$D_{s,i}$	$C_{CN,0}$	$\bar{d}$	$C_{w,i}$	V_i	$C_{0,i}$
10160	700	0	80	30	70	7

variables, and ε is the gaussian noise. the latent variables z and ε follow the gaussian distribution [21], [23]:

$$p(z) = N(z|0, I) = (2\pi)^{-q/2} \exp(-\frac{1}{2}z^T z) \quad (9)$$

$$p(\varepsilon) = N(\varepsilon|0, \sigma^2 I) \quad (10)$$

where σ^2 is the variance of Gaussian noise ε.

The conditional probability distribution of the observed variables under the latent variables is [21], [22]:

$$\begin{aligned} p(x|z) &= N(x|wz + u, \sigma^2 I) \\ &= (2\pi)^{-m/2}(\sigma^2)^{-1/2} \\ &\quad \times \exp(-\frac{1}{2\sigma^2}\|x - wz - u\|^2) \end{aligned} \quad (11)$$

The marginal probability distribution of the observed variables [22], [23]:

$$\begin{aligned} p(x) &= \int_z p(x|z)p(z)dz = N(x|u, ww^T + \sigma^2 I) \\ &= (2\pi)^{-m/2}(ww^T + \sigma^2 I)^{-1/2} \\ &\quad \times \exp\{-\frac{1}{2}(x - u)^T(ww^T + \sigma^2 I)^{-1}(x - u)\} \end{aligned} \quad (12)$$

According to the Bayesian theory [23], the conditional probability distribution of the latent variables under the observed variables:

$$\begin{aligned} p(z|x) &= \frac{p(x|z) * p(z)}{p(x)} \\ &= N(z|v^{-1}w^T(x - u), \sigma^2 v^{-1}) \\ &= (2\pi)^{-q/2}(\sigma^2 v^{-1})^{-1/2} \\ &\quad \times \exp\{-\frac{1}{2}[x - v^{-1}w^T(x - u)]^T \\ &\quad \times (\sigma^{-2}v)[x - v^{-1}w^T(x - u)]\} \end{aligned} \quad (13)$$

where $v = w^T w + \sigma^2 I, v \in R^{q*q}$.

In PPCA model, the model parameters are $\theta = \{w, \sigma^2\}$, which can be optimized iteratively by Expectation Maximum (EM) algorithm [25] when given a train set of the observed variables $x = \{x_1, x_2, \cdots x_n\} \in R^{m*n}$. The log-likelihood function of complete data given by:

$$L(x|\theta) = \ln p(x, z|\theta) = \sum_{i=1}^{n} \ln p(x_i|z_i) + \ln p(z_i) \quad (14)$$

where x_i and z_i are the i-th row of x and z. Substitute (9) and (11) into the above equation, and the posterior probability distribution expectation of latent variables is calculated:

$$\begin{aligned} E(L(x|\theta)) = -\sum_{i=1}^{n}\{&\frac{m}{2}\ln(2\pi\sigma^2) + \frac{1}{2}trace(E(z_i z_i{}^T)) \\ &+ \frac{1}{2\sigma^2}\|x_i - u\|^2 + \frac{1}{\sigma^2}E(z_i)^T w^T (x_i - u) \\ &+ \frac{1}{2\sigma^2}trace(E(z_i z_i{}^T) w^T w) + \frac{q}{2}\ln(2\pi)\} \end{aligned} \quad (15)$$

In the E-step of EM algorithm, the above formula only depends on the posterior probability distribution, which can be calculated as follows [26]:

$$E(z_i) = v^{-1} w^T (x_i - u) \quad (16)$$
$$E(z_i z_i{}^T) = \sigma^2 v^{-1} + E(z_i)E(z_i)^T \quad (17)$$

In the M-step of EM algorithm, keep the posterior statistics fixed, and let the partial derivatives $E(\ln p(x, z|\theta))$ with respect to model parameters w and σ^2 to be zero, the formula of updating model parameters as follows:.

$$w_{new} = [\sum_{i=1}^{n}(x_i - u)E(z_i)^T][\sum_{i=1}^{n}E(z_i)E(z_i)^T]^{-1} \quad (18)$$

$$\begin{aligned} \sigma^2{}_{new} = \frac{1}{nm}\sum_{i=1}^{n}\{&\|x_i - u\|^2 - 2E(z_i)^T w_{new}{}^T \\ &\times (x_i - u) + trace(E(z_i z_i{}^T) w_{new}{}^T w_{new})\} \end{aligned} \quad (19)$$

To summarize, the optimal model parameters can be obtained by iterate alternately (16), (17) and (18), (19) until the model parameters converge. Once given a query sample, the corresponding probability distribution of the latent variables z_q can be calculated by (13).

2) JUST IN TIME LEARNING

To cope with the industrial processes undergo abrupt change characteristics and nonlinearity, just in time learning (JITL) was proposed. It is a local modeling method that has been widely applied in nonlinear modeling, process monitoring and soft sensing [4], [27].

In the JITL framework, when given a query sample x_{new}, it takes the following three steps to predict output [28]: (1) the relevant sample that similar to x_{new} was selected from historical database based on some defined similarity criteria; (2) establish a local model according to the relevant sample sets; (3) the new output y_{new} is predicted with the local model, and then the local model is abandoned [29]- [31]. When the new query data arrives, a new local model will be established on the above procedure [31]. Since a local model is established on selecting a similar data set for each x_{new}, the process characteristics nearby x_{new} can be accurately described, therefore the accuracy and adaptability of the model performance can be greatly improved.

3) PARTIAL LEAST SQUARES

Partial least squares (PLS) is a valid linear modeling method that integrates multivariate statistical regression analysis, canonical correlation analysis, and principal component analysis [32]–[34]. It mainly projects the high-dimensional data space with correlations into mutually orthogonal low-dimensional subspace, and then establishes a linear regression relationship between feature vectors in low-dimensional subspace, which has the advantages of reducing dimension and eliminating the collinearity between variables [32], [34]. Therefore, it has been extensively used in complicate industrial process modeling, monitoring and fault diagnosis [35].

Suppose input is $x = [x_1, x_2, \cdots x_n] \in R^{n*m}$, and the corresponding output is $y = [y_1, y_2, \cdots, y_n] \in R^{n*q}$, which can be expressed the following linear latent variable form [35], [36]:

$$\begin{aligned} x &= \hat{x} + e = tp^T + e \\ y &= \hat{y} + r = uq^T + r \end{aligned} \quad (20)$$

where t and u is the scoring matrix of x and y, p and q is the correspond loading matrix. To extract the maximum variation information between input and output, t and u have the following linear relationship [32], [34]:

$$u = bt + r \quad (21)$$

The PLS regression model is:

$$y = C^{pls} x \quad (22)$$

where r is residual matrix, b is determined by minimizing the residual matrix, $C^{pls} = rbq^T$ is regression coefficient matrix [36].

C. GCLP OPTIMIZATION SETTING COMPENSATION PROBLEM

The optimal economic benefit based on the soft sensor model of the GCLP can be obtained while satisfying the process constraints, which can be described by the following optimization problem:

$$\begin{aligned} &\max\ z = P(y) - C_1(x) - C_2 \\ &s.t.\ \begin{cases} y = f_{pls}(x) \\ y \le a \\ x_{i,D} \le x_i \le x_{i,U} \end{cases} \end{aligned} \quad (23)$$

where x, y, z represents the amount of NaCN, residue gold concentration, overall economic benefit, respectively. P is the product revenue, C_1 is consumption cost, which determined by the consumption of the production. C_2 is the raw material cost, which is usually a constant, $y = f_{pls}(x)$ is the soft sensor model of the GCLP based on PLS, the input of which is $x = [Q_{cn,1}, Q_{cn,2}, Q_{cn,4}]$, and the corresponding output is $y = D_{s,4}$. a is quality index limit value, which is a constant(in this paper $a = 15$). $x_{i,D}$, $x_{i,U}$ are lower and upper boundaries of the i-th ($i = 1, 2, 4$) operating variable, which is determined by process conditions and equipment parameters generally. By solving the above optimization problem (23), it is the optimal setting point x^* that can be obtained in the current GCLP. However, due to model error, the optimal setting point x^* based on the soft sensor model is usually not the optimal working point $x_b{}^*$ of the actual production process. When applying x^* to the actual GCLP, it is difficult to achieve the optimal economic benefit of the actual production process, that is $z(x^*) < z(x_b{}^*)$. To solve this problem, Li K et al proposed a data-based compensation method for optimal setting of hydrometallurgical process [19], which expanding in the vicinity of the optimal setting point x^* obtained based on the model according to Taylor formula [19]:

$$z(x_b{}^*) = z(x^*) + \frac{dz}{dx}(x_b{}^* - x^*) + \delta \tag{24}$$

Deform the above formula:

$$\Delta z = \frac{dz}{dx}(\Delta x) + \delta \tag{25}$$

where $\Delta z = z(x_b{}^*) - z(x^*)$, $\Delta x = x_b{}^* - x^*$, δ is high order infinity.

If the relationship between Δx and $\Delta z (\Delta z = f(\Delta x))$ can be obtained, the compensation value Δx of the current working point can be optimized by solving optimization problem (26). The detailed description please refer to the literature [19], and this paper not be covered.

$$\max_{\Delta x} \Delta z = f(\Delta x)$$
$$s.t. \begin{cases} T^2 \leq \sum \frac{t^2}{s^2} \\ \frac{1}{L-A} \sum (x - \widehat{x})^{\frac{1}{2}} \leq \sigma \\ \Delta x_{i,D} \leq \Delta x \leq \Delta x_{i,U} \\ x_{i,D} \leq \Delta x + x \leq x_{i,U} \end{cases} \tag{26}$$

However, the above method faced two problems: (1) it fails to consider the process data contain noise and uncertainty in the historical database caused by the fluctuation of raw material properties; (2) whether the quality indicator meet the production requirement during each data-based iteration optimization compensation.

III. A DATA-DRIVEN ITERATIVE OPTIMIZATION COMPENSATION METHOD BASED ON PJIT-PLS

To solve the aforementioned problem, this paper propose a data-driven iterative optimization compensation method that under the premise of quality indicator meet the requirement, utilizing the data-based and local model-based technique, keeping x^* constantly close to the optimal working point $x_b{}^*$ of the actual production process, thereby improving the economic benefit. Specifically: firstly the optimal setting point x^* on the basis of the soft sensor model for GCLP and the corresponding economic benefit $z_m(x^*)$ can be obtained through solve the problem (23), and apply x^* to the actual GCLP through the control layer to gain the actual economic benefit $z_a(x^*)$; Secondly, Compares $z_m(x^*)$ and $z_a(x^*)$, data-driven iterative optimization compensation method is required only if $z_m(x^*) < z_a(x^*)$, otherwise no needed; Finally, PPCA technique is used to preprocess the process data and that similar to the current optimal setting point x^* from the historical database can be selected by JIT, and then establish the relationship model between the operating variable increment Δx and the economic benefit increment Δz, the residue gold concentration increment Δy based on PLS, respectively. The optimal compensation value Δx can be gained and implement $x^* + \Delta x$ as a new working point through the control layer to the actual GCLP. By iteratively updating the compensation value Δx, the economic benefit of GCLP have also been constantly improved. The specific data-driven iterative optimization compensation process as shown in Fig. 2.

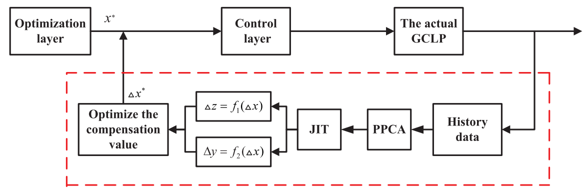

FIGURE 2. Structure diagram of data-driven iterative optimization compensation process.

A. MODELING BASED ON PJIT-PLS

To handle data noise and uncertainty effectively, this paper proposes a PJIT-PLS method: Firstly, the historical samples are preprocessed by PPCA modeling method, and the posterior Gaussian distribution of the low-dimensional latent variables of the samples can be obtained; Secondly, once the query data x_q arrives, the posterior probability of the latent variable of which can be obtained by the trained PPCA model, and the Symmetric Kullback-Leibler-based (SKL-based) as similarity measurement criterion that evaluating the dissimilarity Gaussian distributions between the query sample and the historical samples, and then the similar data sets can be selected; Finally, based on the PLS modeling method, two models are built using selected similar data sets. The framework of the proposed PJIT-PLS method as shown in Fig. 3. The specific process as follows:

(1) Data preprocessing: to eliminate process data noise and uncertainty due to the fluctuation of initial gold concentration in the ore of the actual GCLP. Historical data sets $x = \{x_1, x_2, \cdots x_n\} \in R^{n*m}$ are trained by PPCA, model parameters set $\theta = \{w, \sigma^2\}$ and the posterior probability of the latent variable $N(z_j|u_j, \sigma_j{}^2)(j = 1, 2, \cdots n)$ can be obtained. When a query sample arrives, the corresponding posterior probability of the latent variable $N(z_q|u_q, \sigma_q{}^2)$ can be estimated directly using (13).

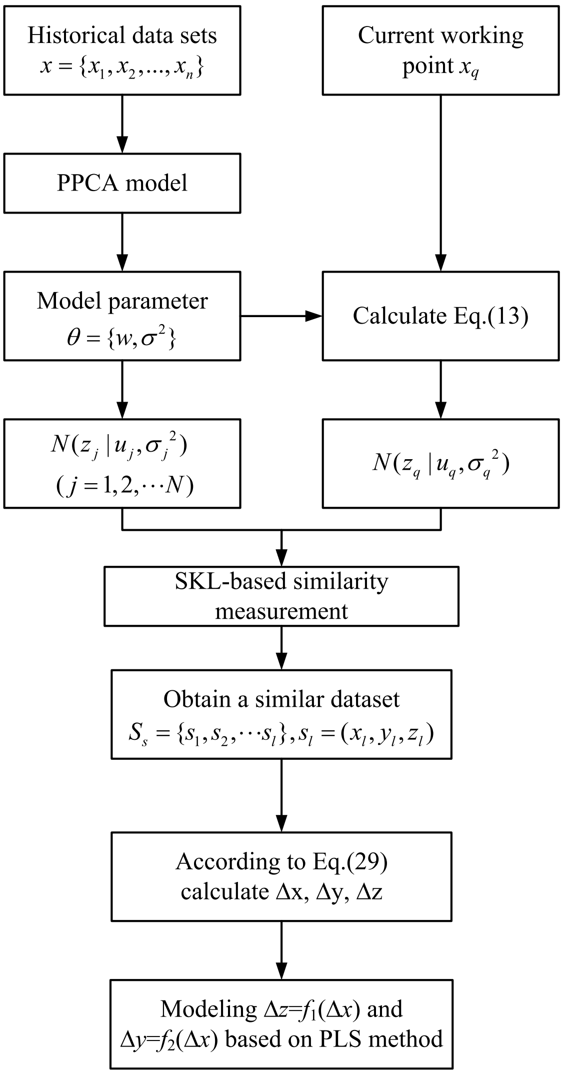

FIGURE 3. Framework of the proposed PJIT-PLS method.

(2) Similarity metric for selecting similar samples: the most important factor to a successful JITL is to choose suitable similarity criteria that select the most appropriate relevant samples from history database for local modeling. Many of them have been put forward, like the distance-based [27]- [28], angle-based [29], [30], [37], correlation-based [38], [39] similarity criteria. The traditional similarity measurement method that measuring point-to-point is no longer applicable because it is now measuring two Gaussian probability distribution. Therefore, a new similarity measurement method that SKL-based should be adopted to measure the similarity between the Gaussian probability distribution of latent variables [21], [40], which is defined as follows:

$$\begin{aligned} SKL(q,j) &= D_{skl}[N(z_q|u_q,{\sigma_q}^2), N(z_j|u_j,{\sigma_j}^2)] \\ &= \frac{1}{2} * \{trace[({\sigma_q}^2-{\sigma_j}^2)(({\sigma_q}^2)^{-1}-({\sigma_j}^2)^{-1})] \\ &\quad + [(u_q-u_j)^T(({\sigma_q}^2)^{-1}+({\sigma_j}^2)^{-1})(u_q-u_j)]\} \\ &\qquad (j=1,2,\cdots N) \end{aligned} \tag{27}$$

$$S_i = \exp(-\frac{SKL_i}{SKL_{\max}})(i=1,2,\cdots N) \tag{28}$$

The bigger $S_i(S_i \in (0,1))$, the more similar between query sample and history sample, and vice versa. The procedure of picking similar data sets: firstly calculating SKL values that is the Gaussian probability distribution of latent vector between query sample and historical samples, then utilizing (28) calculate S_i, at final, a similar data sets can be obtained according to a similarity threshold $\xi(S_i \geq \xi)$, in this paper $\xi = 0.85$. Compared to traditional similarity measures deterministic point-to-point, SKL-based similarity measurement method can pick more similar data sets by measuring the dissimilarity between Gaussian probability distribution of two latent vectors. The relevant simulation verification will be given in Section4.

(3) Online Local Modeling: the production information of the current working condition is $S_q = (x_q, y_q, z_q)$, x, y, z represent the corresponding operating variables, the quality index and the economic benefit, respectively. A similar data set $S = \{(x_1, y_1, z_1), (x_2, y_2, z_2), \cdots, (x_l, y_l, z_l)\}$ can be selected according to the SKL-based method, l is the number of selecting similar samples. Subtracting from similar samples with current working condition:

$$\begin{aligned} \Delta x_i &= x_i - x_q \\ \Delta y_i &= y_i - y_q \\ \Delta z_i &= z_i - z_q (i=1,2,\cdots,l) \end{aligned} \tag{29}$$

For simplicity $\Delta x = \{\Delta x_1, \Delta x_2, \cdots \Delta x_l\}$, $\Delta y = \{\Delta y_1, \Delta y_2, \cdots \Delta y_l\}$, $\Delta z = \{\Delta z_1, \Delta z_2, \cdots \Delta z_l\}$. Based on PLS method, establishing two local models $\Delta z = f_1(\Delta x)$ and $\Delta y = f_2(\Delta x)$.

B. SOLVE THE OPTIMAL SETTING COMPENSATION VALUE ΔX

$$\max_{\Delta x} \Delta z = f_1(\Delta x) \tag{30}$$
$$s.t.\ \Delta y = f_2(\Delta x) \tag{31}$$
$$y_0 + \Delta y \leq 15 \tag{32}$$
$$T^2\_D_{f_1,f_2} \leq T^2 \leq T^2\_U_{f_1,f_2} \tag{33}$$
$$SPE\_D_{f_1,f_2} \leq SPE \leq SPE\_U_{f_1,f_2} \tag{34}$$
$$x_{i,D} \leq \Delta x + x \leq x_{i,U} \tag{35}$$

Utilizing two local models $\Delta z = f_1(\Delta x)$ and $\Delta y = f_2(\Delta x)$ solve the above optimization problem. In order to ensure the optimization solution so far as practicable, which need to satisfy the above constraints. Where (31)-(32) ensure that the quality indicator satisfy the production requirement once the iterative optimization compensation is completed, y_0 is the residue gold concentration at the current working point; Meanwhile, to ensure that within the effective range of the modeling data, the (33)-(34) must be satisfied, $T^2\_D_{f_1,f_2}$ and $T^2\_U_{f_1,f_2}$ represent the upper and lower limits of T^2 statistics for both models, $SPE\_D_{f_1,f_2}$ and $SPE\_U_{f_1,f_2}$ represent the upper and lower limits of SPE statistics for both local models [31] respectively. Due to the limitations of the

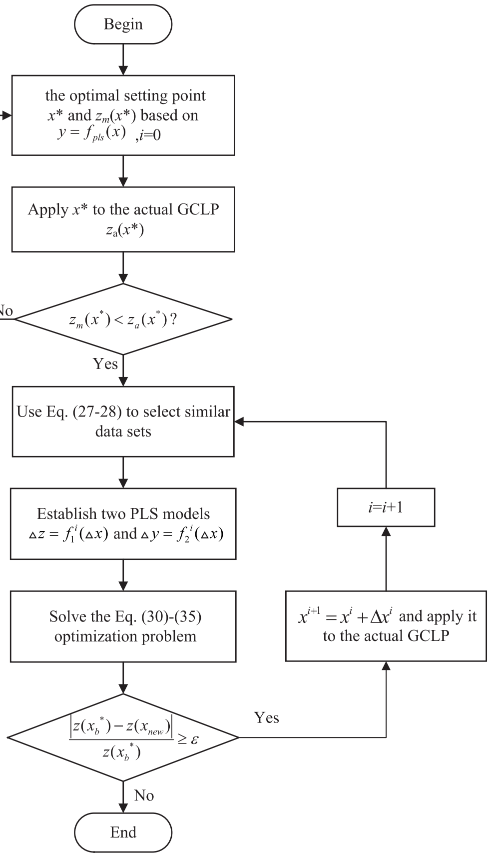

FIGURE 4. **Flowchart of iterative optimization settings compensation method.**

process conditions and equipment parameters of the entire GCLP, it is necessary to ensure that every operating variable in the lower and upper range after each iterative optimization compensation process, the (35) are required to be satisfied. The compensation value optimized by the above optimization problem, and apply $x_{new} = x + \Delta x$ to the actual GCLP through the control layer, the corresponding economic benefit $z(x_{new})$ can be obtained. At this point, the production process working at a new working point, economic benefit increasing gradually. The iterative optimization compensation process for setting point continues in the same manner until (36) is not satisfied (in this paper, $\varepsilon = 0.005$) and the iterative optimization compensation process stops.

$$\frac{|z(x_b{}^*) - z(x_{new})|}{z(x_b{}^*)} \geq \varepsilon \tag{36}$$

In summary, the flow chart of iterative optimization compensation process is shown in Fig. 4.

The steps of data-driven iterative optimization compensation process as follows:

Step1: Based on the soft sensor model $y = f_{pls}(x)$ of GCLP, the optimal operating variables x^* and corresponding economic benefit $z_m(x^*)$ can be optimized by (23), $i = 0$;

Step2: Apply x^* to the actual GCLP through the control layer and calculate the corresponding economic benefit $z_a(x^*)$;

TABLE 3. **The parameter settings of the PSO algorithm.**

Parameter items	Value
Population size	100
Maximum number of iterations	100
Learning factors	$c_1(t) = 2.5 - 2.0 * t/100$ $c_2(t) = 0.5 + 2.0 * t/100$
Inertia weights	$w(t) = 0.5 * (100 - t)/100 + 0.4$

Step3: If $z_m(x^*) < z_a(x^*)$, the iterative optimization compensation method is required, go to step4, otherwise, returns to step1, and keep the current economic benefit $z_m(x^*)$;

Step4: Select relevant data sets that similar to $(x^*, z_m(x^*))$ according to (27)-(28);

Step5: Establish the relationship model between Δy, Δz and Δx respectively, that is $\Delta z = f_1{}^i(\Delta x)$ and $\Delta y = f_2{}^i(\Delta x)$ by using PLS method;

Step6: Solve the optimization problem (30)-(35), Δx^i can be obtained and apply $x^{i+1} = x^i + \Delta x^i$ to the actual GCLP through the control layer, $i = i + 1$;

Step7: If (36) is satisfied, returns to Step4, otherwise, ends.

IV. SIMULATION AND RESULTS

In this section, the effectiveness of the proposed data-driven iterative optimization compensation method based on PJIT-PLS was validated in the simulation studies of GCLP. To validate the superiority of the PJIT-PLS and SKL-based similarity measurement method, deterministic JIT-PLS (DJIT-PLS) approach [19] is carried out for compensation effect comparison in terms of iterations and improve the economic benefit.

Using the mechanistic model $y = f_m(x)$ for GCLP as the simulated reality, and the data-driven model $y = f_{pls}(x)$ is used as the soft sensor model. Applying particle swarm optimization (PSO) algorithm solve the optimal setting point x^* of the soft sensor model and the corresponding economic benefit $z_m(x^*)$ as well as quality index $y_m(x^*)$ can be gained. The parameter settings of the PSO algorithm are shown in Table 3 (t represents $t - th$ iteration, $t \in [1, 100]$ and $t \in Z$).Then bring the optimal setting point x^* into the mechanistic model that simulates the actual production process, and the corresponding economic benefit $z_a(x^*)$ and quality index $y_a(x^*)$ can be calculated. Meanwhile, PSO is used to solve the optimal working point $x_b{}^*$ of the mechanistic model and obtain the corresponding economic benefit $z_b(x^*)$ and quality index $y_b(x^*)$. The optimization results based on the mechanistic model and the soft sensor model is shown in Table 4, the sum consumption of the optimal operating variables based on the soft sensor model is much larger than that based on the mechanistic model, and the combination order has changed, which leads to lower economic benefit.

According to the simulation results $z_a(x^*) = 4388.89$ (¥$/h$), data-driven iterative optimization compensation process is required. The mechanistic model is used as the simulated reality to randomly generate 1000 groups data (x_h, y_h, z_h) as historical datasets. Based on the proposed

TABLE 4. The optimization results.

Variables name	Soft sensor model	Mechanistic model
$Q_{cn,1}$ kg/h	13.41	28.17
$Q_{cn,2}$ kg/h	15.63	19.15
$Q_{cn,4}$ kg/h	72.134	16.78
$sum(Q_{cn})$ kg/h	101.17	64.10
y mg/kg	14.67	14.90
z ¥/h	4180.57	4629.32

TABLE 5. Compensation result for each iteration.

Number of iterations	1	2	3
$\Delta Q_{cn,1}$ kg/h	12.43	-0.91	5.77
$\Delta Q_{cn,2}$ kg/h	-8.99	5.55	8.30
$\Delta Q_{cn,4}$ kg/h	-16.70	-19.31	-21.63
Δy mg/kg	-0.24	0.20	0.19
y mg/kg	14.43	14.63	14.82
Δz ¥/h	188.17	171.93	82.02
z ¥/h	4368.74	4540.63	4622.70

TABLE 6. The optimal values and the operation after compensation.

Variables name	Mechanistic model	After compensation
$Q_{cn,1}$ kg/h	28.17	30.70
$Q_{cn,2}$ kg/h	19.15	20.50
$Q_{cn,4}$ kg/h	16.78	14.48
$sum(Q_{cn})$ kg/h	64.10	65.68
y mg/kg	14.90	14.82
z ¥/h	4629.32	4622.70

PJITL-PLS approach, historical datasets was preprocessed by PPCA, then l groups similar data $(x_i, y_i, z_i)i = 1, 2, \ldots, l$ is selected from the historical data set by (27) and (28), and then the difference information can be obtained by subtracting similar data with the current production information $(x^*, y_a(x^*), z_a(x^*))$ respectively, and establish $\Delta z = f_1{}^i(\Delta x)$ and $\Delta y = f_2{}^i(\Delta x)$ based on PLS method. The same PSO algorithm is used to solve the optimization problem (30)-(35). After three iterations compensation, the (36) is no longer satisfied, the iterative optimization compensation process stops. The information of which $(\Delta x, \Delta y, \Delta z)$ is shown in Table 5.

As shown in Table 6, after undergo three iterations compensation, the operating variables at the new work point is close to the optimal working point of the actual GCLP, and the order of which in accord with the optimal operating variables. Meanwhile, the total consumption of operating variables also similar extremely so as to improve economic efficiency greatly.

As shown in Fig. 5, the production process begins at the initial optimal setting point, and the economic benefit is 4180.57(¥/h), utilizing data-driven iterative optimization compensation method for compensate the current working point, the economic benefit value is stable around the optimal value after three iterations compensation, production process runs at new working point, and the economic benefit reaches 4622.70(¥/h), which improved by 10.57%. Specially, during the compensation process of three iterations, the quality index satisfy production requirement (residue gold concentration $\leq$ 15).

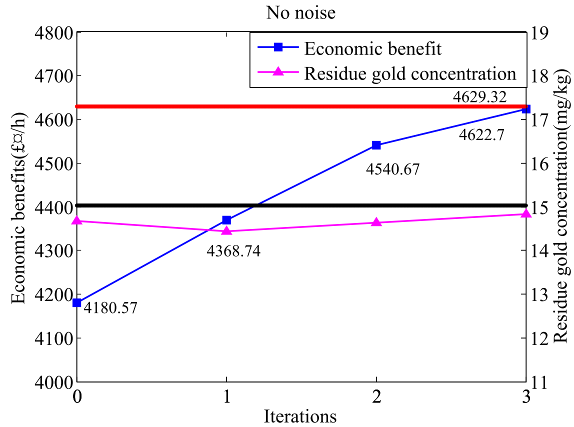

FIGURE 5. Iterative compensation results based on based on the optimization problem (30)**.**

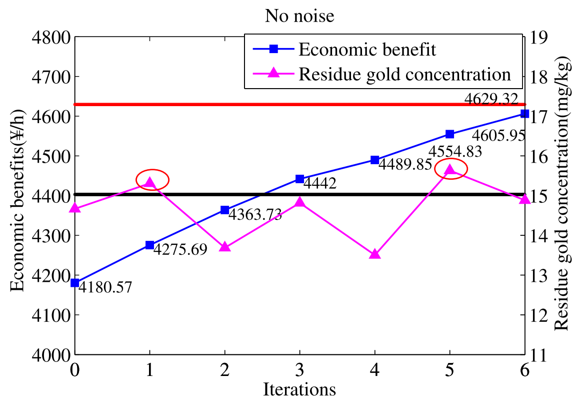

FIGURE 6. Iterative compensation results based on the optimization problem (26)**.**

The optimization problem (26) was used to optimize the GCLP, the simulation results are shown in the Fig. 6. The similar samples are selected from the historical datasets based on combine Euclidean distance with angle for PLS modeling, which method was referred to DJIT-PLS in this paper. After six iterations compensation, production process runs at new work point, and the economic benefit reaches 4605.95(¥/h), which improved by 10.18%. Specially, in the first and fifth compensation, the residue gold concentration exceeds the production requirement (15mg/kg), which is not allowed in the actual production process. Compared with the Fig. 5, the method proposed in this paper can iterative optimization compensation on the premise that the quality index meet the requirements, which owing to the quality index (31)-(32) to be constrained when data-driven iterative optimization compensation is carried out. At the same time, with the rapid development of modern industry, the flow control can be switched freely, there is no need to restrict whether the compensation operating values meets its upper and lower bounds, as long as the operating variables after compensation within upper and lower bounds individually. Therefore, this paper proposed a data-driven iterative optimization compensation method under the condition of the quality index meet the

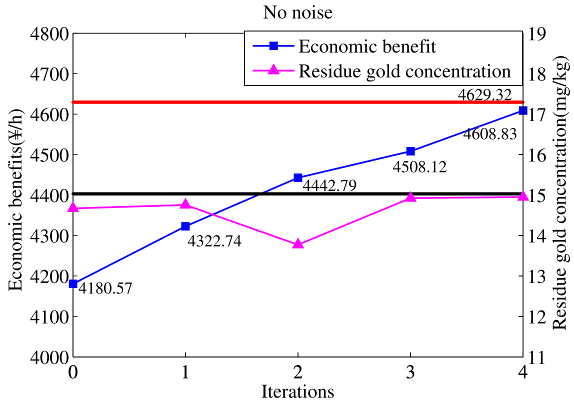

FIGURE 7. Iterative compensation results based on DJITL-PLS.

TABLE 7. Comparison of compensation results for two methods under no noise.

Number of iterations	PJIT-PLS(¥/h)	DJIT-PLS(¥/h)
1	4368.74	4322.74
2	4540.67	4442.79
3	4622.70	4508.12
4	-	4608.83

production requirement is verified by comparing the simulation results.

Solve the optimization problem (30)-(35) based on DJITL-PLS method, the simulation results are shown in the Fig. 7. After four iterations compensation, production process runs at new work point, and the economic benefit reaches 4608.83(¥/h), which improved by 10.24%. Compare Fig. 5 with Fig. 7, we can draw the conclusion that the method has the advantage of the quality indicator meet the production requirements in the iterative compensation process and has fewer iterations compare with the optimization problem (26).

When the historical dataset with no noise, PJIT-PLS and DJIT-PLS methods were used for modeling respectively, and then solving the optimization problem (30)-(35).The compensation results of two methods as shown in Table 7, the proposed method has the advantages of fewer iterations and more economic benefit because that SKL-based method was used as similarity criterion to select similar samples appropriately, which enables JIT to be successfully applied in this paper.

The noise with Gaussian distribution of 2% standard deviation are added to the initial gold concentration in the ore $D_{s,0}$, by solving the optimization problem (30)-(35), the iterative compensation results of PJIT-PLS and DJIT-PLS as shown in Fig. 8 and Fig. 9. Applying PJIT-PLS to establish two model, and which was used to optimize the production process. After three iterations compensation, the economic benefit were improved by 439.47(¥/h), while DJIT-PLS require five iterations compensation, the economic benefit are improved by 433.48(¥/h). PJIT-PLS has the advantage of fewer iterations and higher economic benefit. The main reason is that the historical datasets and current working point was PPCA technology preprocessed, and then the latent variable distribution of the corresponding sample was obtained and SKL-based similarity criterion was used to

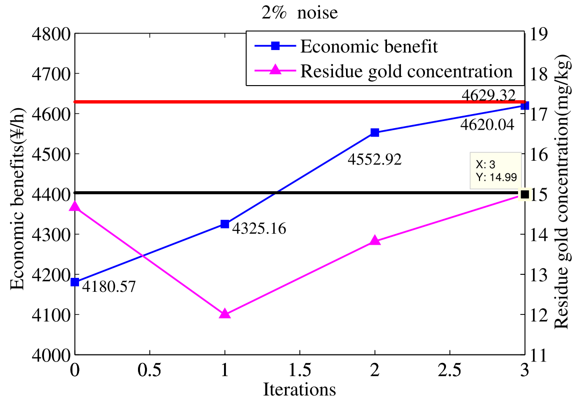

FIGURE 8. Iterative compensation results based on PJITL-PLS under 2% noise.

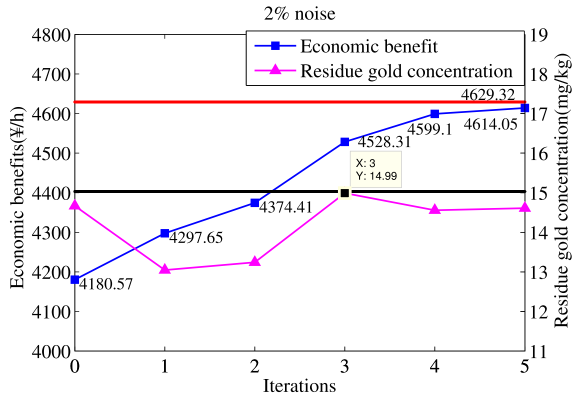

FIGURE 9. Iterative compensation results based on DJITL-PLS under 2% noise.

select similar samples, thereby eliminates the effect of data noise and uncertainty. The comparative simulation results show that the proposed method can effectively overcome the problem caused by the fluctuation of raw material properties.

V. CONCLUSION

In this work, a data-driven iterative optimization compensation strategy was proposed to solve the problem that the method of model-based is difficult to achieve the optimal economic benefit of the actual GCLP as well as process data contains noise and uncertainty due to the fluctuations of initial gold concentration in the ore. Firstly, PJIT-PLS method was proposed to establish two relevant models between operating variables increment and the economic benefit increment, the quality index increment in the vicinity of the optimal setting point based on soft sensor model; Secondly, the optimal operating variables increment can be optimized under the condition of quality index satisfy the production requirement and iterated compensate at the new working point, which constantly close to the optimal working point of the actual process in order to effectively improve the economic benefit of the production process; Lastly, simulation studies was performed in a simulated GCLP to verify the validity of proposed method.

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