

Product Quality Modeling and Optimizing Control of Soft Capsule Dropping Pills Based on LSSVM and PSO

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Abstract—Soft capsule dropping pills product quality control system is a multi-input and multi-output complex system. First of all, the process parameters and a two-level hierarchy index system of soft capsule pills product quality were proposed based on the analysis to the production process. Then the model was established based on least squares support vector machine (LSSVM), whose inputs are the process parameters and outputs are the secondary quality indexes. Analysis hierarchy process (AHP) was used to determine the weights of the secondary quality indexes. On this basis, particle swarm optimization (PSO) algorithm was used to optimize the process parameters in order to improve the yield of soft capsule pills, which is a multi-objective optimization problem. The nominal values of the process parameters corresponding to the highest yield can be obtained. The yield increases by 2.7% when the optimizing parameters are used to the soft capsule dropping pills process.

I. INTRODUCTION

IN the manufacturing and processing production line, product quality control problems are focus of extensive attention in industry and the academic circles at home and abroad. Over the past, the online detection of product quality and process parameters are very difficult due to the lack of effective means of online testing. With the development of the intelligent modeling and soft-sensing methods, product quality on-line control has become possible, and has gradually become an important direction of the industrial production development [1]. This work is to study the product quality optimization of soft capsule pills pharmaceutical production process based on such considerations.

Aiming at the large-scale industrial systems product quality control and optimization problem, The team led by Professor Wan of Xi'an Jiaotong University conducted an in-depth research and made a series of results [1-3]. The product quality model and quality control model of the industrial production

were put forward in [2]. The flash furnace production process and product quality model based on neural network technology were founded, and steady-state optimizing control problem of flash furnace was studied in [3]. A dynamic optimization method based on product quality driven was proposed and used in baking processes in [4]. The product quality modeling and control methods based on machine vision was studied and used in baking processes in [5].

In [6], artificial neural networks were applied to the pilules manufacturing process modeling, and genetic algorithm was used to optimize the input technological parameters of the model for improving the yield of the pilules. The pilules are solid balls, which are different from the soft capsules dropping pills, and genetic algorithm was used to a single goal optimization. However, the product quality problems are usually multi-objective optimization problem. So the optimization method has to be further improved.

Soft capsule dropping pills is a method to produce seamless capsules for cod liver oil pharmaceutical industries. The basic principle is that the gelatin solution and the medical solution form a concentric flow column through the emitter. The flow column is cut into paragraphs evenly by liquid pulse, and then the paragraphs enter the paraffin oil circulatory system for cooling, while the spherical capsules are formed with the effect of gelatin solution surface tension [7].

The method has the advantages of simple process, low-cost production equipment, low loss and quick drugs effect compared with other pharmaceutical methods. However, because of the pills are formed through the specific dripping system, and therefore the quality is very sensitive to changes of process parameters. Especially the appearance quality indexes, are more susceptible to the above mentioned process parameters change. The strong nonlinear and coupling are existed between process parameters and quality indexes. It is difficult to establish an effective quality control model by using traditional methods. The production control relies on the experience to a great extent, so it is difficult to guarantee the stability of the quality, and the yield need to be further improved.

Considering the characteristics of dropping pills production process, first of all, the model of soft capsule dropping pills based on least squares support vector machine (LSSVM) was

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established, whose inputs are technological parameters and outputs are the secondary quality indexes. Then use the samples collected from the experiment and production process for training the model, which determines the mapping relations between the process parameters and the product quality indexes. Finally the particle swarm optimization (PSO) algorithm with global search capabilities is used to optimize the model input parameter space, whose ultimate goal is to improve the yield of soft capsule pills. The nominal value of technological parameters corresponding to the highest yield can be obtained, which can be used to guide the production, and improve the yield.

The paper is organized as follows. At first, an introduction is given in Section I. Section II presents the mathematical model of soft capsule dropping pills based on LSSVM, In Section III, PSO algorithm is introduced with a use to optimize the input process parameters, while a detailed discussion is provided in Section IV. Finally, we conclude the paper with some remarks in Section V.

II. SOFT CAPSULE DROPPING PILLS PRODUCT QUALITY MODELING

The traditional system modeling method is the use of people's understanding of physical processes, through the mechanism analysis to set up the structure model of the system, and then use the observed data to estimate model parameters. For linear system or the essential linear system, this method is relatively effective. But for complex nonlinear systems, it is very difficult to set up an accurate system model by using this traditional method of modeling, so the data-driven modeling method needs to be taken.

A. Select the Input Process Parameters

There are many kinds of process parameters involved in the soft capsule dropping pills forming process, which have different impact degrees on product quality. So in order to improve the efficiency and reduce the complexity of the model, the parameters selection of the modeling process will follow the following principles [7]:

1) The selected input process parameters must be easy to control. The grasp of the standard is mainly from the perspective of the project implementation.

2) The selected input process parameters are independent of each other, which can be selected using statistical analysis.

3) The selected input process parameters should have significant effect on output the quality indexes. On the one hand, correlation analysis is used to search process parameters, which have significant impact on the quality indexes; on the other hand, expertises are used in the selection of process parameters.

In accordance with these principles, the four process parameters were selected as input variables for LSSVM

modeling, namely gelatin solution viscosity x_1 , gelatin solution temperature x_2 , paraffin oil temperature x_3 , and pulse pressure x_4 . The output variables of the model are four secondary indexes, respectively as spherical degree y_1 , tailed degree y_2 , breaking pill rate y_3 , and collodion silk degree y_4 ; whose values are at $[0,5]$, the bigger the better. The yield is the first grade index, which are determined by the four secondary quality indexes.

B. Modeling Data Collection and Processing

In this paper, the data for modeling are from the original experimental data of soft capsule dropping pills. It is because the operator has experience on the other form of soft capsule dropping pills machine, so we designed a more reasonable test scope on the choice of experimental data combined with empirical data in the past, which reduced the scope of selection and shortened the feeling time, reduced the blindness of the experiment, and improved the efficiency. We adopted orthogonal test method for their selection, and ultimately won the 80 experimental data samples.

There are many process parameters inspection point in the production process, and the process parameters have different units of measure, even if some of the parameters have the same unit of measurement, the changes scope of the measured values are different, sometimes the difference is relatively large. For example, the paraffin oil temperature is generally at around 10 °C, and the gelatin solution temperature is typically up to tens of Celsius degrees, the viscosity of gelatin solution is at a few hundred or even more than 1000cp, and the values of spherical degree y_1 , tailed degree y_2 , breaking pill rate y_3 and collodion silk degree y_4 are at $[0,5]$. If the collected data are used directly for data analysis modeling, it will exaggerate the role of the larger dimension parameters, and conceal the actual changing relationship between the various parameters, that is, have a so-called false variation. Therefore, before the raw data are used into the analysis, it is necessary to deal with them in order to eliminate the effect of variable dimensions to the modeling. In this paper, the smallest - the largest is the way to transform all data to standardized interval $[0,1]$. The transformation formula is as follows:

$$y' = \frac{y - y_{\min}}{y_{\max} - y_{\min}}, \quad (1)$$

where y, y' are the data before and after normalization, y_{\min}, y_{\max} are the minimum and maximum sampling data of the corresponding variables.

The sample set composed of 80 data samples is divided into two parts after pretreatment and normalization, and denoted by sample sets S_1 and S_2 , respectively. S_1 is for training and modeling, which composed of 60 records; S_2 is the test sample set, with 20 records. After training, the nonlinear expression of

mathematical models can be obtained for spherical degree y_1 , tailed degree y_2 , breaking pill rate y_3 and collodion silk degree y_4 . The soft-sensing models are achieved.

C. Function Estimate Using Least Squares Support Vector Machine[8]

Consider a given set of training sample $D = \{(x_k, y_k) | k = 1, 2, \dots, N\}$, where, N denotes the number of samples, $x_k \in R^n$ are the input data, and $y_k \in R$ are the output data. Suppose the regression function as

$$y(x) = w^T \phi(x) + b \quad (2)$$

Where w is a weight vector in the feature space. $b \in R$ is the deviation.

The introduction of structural risk function will return the regression issue into the following optimization problem.

$$\min J = \min \left(\frac{1}{2} w^T w + \gamma \frac{1}{2} \sum_{k=1}^n e_k^2 \right) \quad (3)$$

The constraint is described as:

$$y_k = w^T \phi(x_k) + b + e_k, k = 1, \dots, n. \quad (4)$$

Where $\phi(\cdot)$ stands for nonlinear transform function, which transform the input space into high-dimensional space, e denotes relaxation item, γ denotes punishment item for the error.

The corresponding Lagrangian function is as follows:

$$L(w, b, e, \alpha) = J(w, e) - \sum_{k=1}^n \alpha_k \{w^T \phi(x_k) + b + e_k - y_k\}, \quad (5)$$

where $\alpha_k \in R$ represents Lagrangian multipliers. From the KKT theorem [8]:

$$\begin{aligned} \frac{\partial L}{\partial w} = 0 &\rightarrow w = \sum_{k=1}^n \alpha_k \phi(x_k), \\ \frac{\partial L}{\partial b} = 0 &\rightarrow \sum_{k=1}^n \alpha_k, \\ \frac{\partial L}{\partial e_k} = 0 &\rightarrow \alpha_k = \gamma e_k, \\ \frac{\partial L}{\partial \alpha_k} = 0 &\rightarrow w^T \phi(x_k) + b + e_k - y_k = 0, \end{aligned} \quad (6)$$

for $k = 1, \dots, n$, eliminate the w and e , linear equations are described as

$$\begin{bmatrix} 0 & \bar{1}^T \\ \bar{1} & Z Z^T + \gamma^{-1} I \end{bmatrix} \begin{bmatrix} b \\ \bar{\alpha} \end{bmatrix} = \begin{bmatrix} 0 \\ Y \end{bmatrix}, \quad (7)$$

where, $Z = [\phi(x_1)^T y_1, \dots, \phi(x_N)^T y_N]$, $Y = [y_1, \dots, y_n]$, $\bar{1} = [1, \dots, 1]$, $e = [e_1, \dots, e_n]$, $\bar{\alpha} = [\alpha_1, \dots, \alpha_n]$, I stands for a unit matrix.

According to the Mercer conditions, the following equality holds [9]:

$$\Omega_{kl} = y_k y_l \phi(x_k)^T \phi(x_l) = y_k y_l K(x_k, x_l) \quad (8)$$

Therefore, the linear equations can be rewritten as:

$$\begin{bmatrix} 0 & \bar{1}^T \\ \bar{1} & \Omega + \gamma^{-1} I \end{bmatrix} \begin{bmatrix} b \\ \bar{\alpha} \end{bmatrix} = \begin{bmatrix} 0 \\ Y \end{bmatrix}. \quad (9)$$

The non-linear regression function is described as:

$$y_k = \sum_{j=1}^n \alpha_j K(x_j, x_k) + b, \quad (10)$$

where, α and b are the solutions of (9).

Thus, despite the sample data are mapped to a high dimensional or even the infinite dimensional feature space by a nonlinear function, the nonlinear function does not require explicit calculation in calculating the regression function. And only the kernel function needs to be calculated, which avoid “curse of dimensionality” problem caused by the high dimensional feature space [10].

D. Design and Implement of LSSVM Based Modeling

After training to the input variables and output variables, the nonlinear expression of mathematical models can be obtained for the four subquality model, spherical degree y_1 , tailed degree y_2 , breaking pill rate y_3 and collodion silk degree y_4 .

$$y_1 = f_1(x_1, x_2, x_3, x_4), \quad (11)$$

$$y_2 = f_2(x_1, x_2, x_3, x_4), \quad (12)$$

$$y_3 = f_3(x_1, x_2, x_3, x_4), \quad (13)$$

$$y_4 = f_4(x_1, x_2, x_3, x_4). \quad (14)$$

Where, $f_1 - f_4$ are the non-linear functions of regression estimator.

In the LSSVM modeling, we choose RBF kernel

$$K(x, x_i) = \exp \left\{ -\frac{\|x - x_i\|^2}{\sigma^2} \right\} \quad (15)$$

as a kernel function of SVM. The RBF kernel has good performance in general smoothness assumption [11]. In order to increase the reliability of the experimental results, the parameters optimization in LSSVM is solved by cross-validation methods.

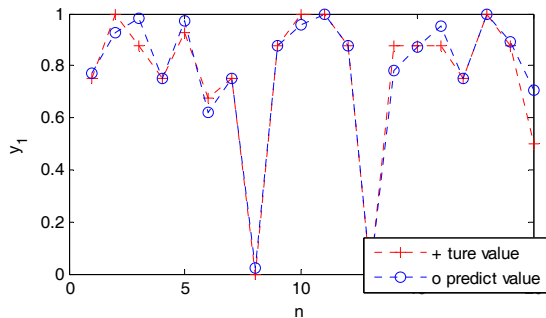


Fig. 1. Comparisons of prediction values and real values of spherical degree y_1

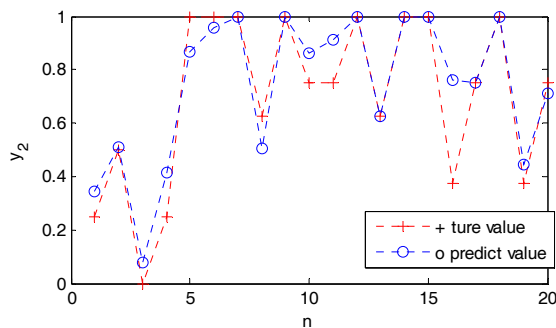


Fig. 2. Comparisons of prediction values and real values of tailed degree y_2

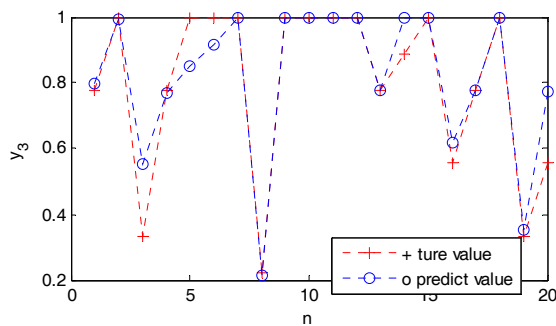


Fig. 3. Comparisons of prediction values and real values of breaking pill rate y_3

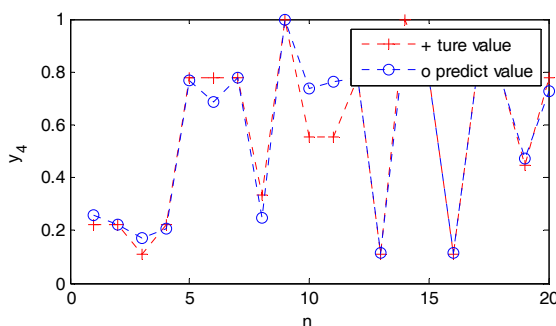


Fig. 4. Comparisons of prediction values and real values of collodion silk degree y_4

Through training, the four soft capsule pills quality learning curves are obtained. The running curves and learning curves for spherical degree y_1 , tailed degree y_2 , breaking pill rate y_3 and collodion silk degree y_4 are shown in Fig. 1 – 4.

The simulation results indicate the predict curves of the models based on LSSVM run close to the actual curves, have high fit accuracy and good generalization ability and meet the modeling requirements.

It can be inferred that when all process parameters are inspected, the model will be shown as a multidimensional mapping surface between the input and output. One optimizing point will exist in the surface, which are the best nominal process parameters.

III. SOFT CAPSULE DROPPING PILLS PRODUCT QUALITY OPTIMIZING CONTROL

In this paper, according to the characteristics of the soft capsule pills process product quality model, PSO algorithm is used for the multi-objective optimization problem of product quality control. A linear weighted sum method is used to transform the multi-objective optimization model into a single objective optimization model. The weights of the indexes are determined by AHP method. The judgment matrix is determined based on the experiences of the experts and experienced operators. The practice has proved that the method is practicable.

A. An Introduction to Particle Swarm Optimization

The Particle Swarm Optimization (PSO) is a swarm intelligence method that models social behavior to guide swarms of particles towards the most promising regions of the search space. PSO has proved to be efficient at solving unconstrained global optimization and engineering problems. It is easily implemented, using either binary or floating point encoding, and it usually results in faster convergence rates than the genetic algorithms [12]. In view of the above mentioned characteristics of PSO algorithm, this paper use PSO algorithm to optimize the process parameters.

At first, let us define the notation adopted in this paper: assuming that the search space is D-dimensional, the i -th particle of the swarm is represented by the D-dimensional vector $X_i = (X_{i1}, X_{i2}, \dots, X_{iD})$, and the best particle in the swarm, i.e. the particle with the smallest function value, is denoted by the index g . The best previous position (i.e. the position giving the best function value) of the i -th particle is recorded and represented as $P_i = (P_{i1}, P_{i2}, \dots, P_{iD})$, while the position change (velocity) of the i -th particle is represented as $V_i = (V_{i1}, V_{i2}, \dots, V_{iD})$. Following this notation, the particles are manipulated according to the following equations

TABLE I
THE PAIRWISE COMPARISON SCALE

Intensity of Importance	Definition
1	equal importance both element
3	weak importance one element over another
5	essential or strong importance one element over another
7	demonstrated importance one element over another
9	absolute importance one element over another
2, 4, 6, 8	intermediate values between two adjacent judgments
reciprocal	a_i compare with a_j is a_i / a_j , then a_j compare with a_i is a_j / a_i

$$V_i^{n+1} = w \cdot V_i^n + c_1 \cdot r_{i1}^n \cdot (P_i^n - Y_i^n) + c_2 \cdot r_{i2}^n \cdot (P_g^n - Y_i^n) \quad (16)$$

$$Y_i^{n+1} = Y_i^n + V_i^{n+1} \quad (17)$$

where $d = 1, 2, \dots, D$; N is the size of the population; $i = 1, 2, \dots, N$; w is the inertia weight; c_1 and c_2 are two positive constants; r_{i1} and r_{i2} are two random numbers within the range $[0, 1]$.

B. Calculate the Weights of the Indexes

The weight of the index is a quantitative indicator of the relative importance of that. In this paper, all the weights are determined by analytic hierarchy process (AHP) method. The specific process using AHP method to determine the weight of the index is as follows [13]:

1) *Establish Each Factor of the Pair-wise Comparison Matrix*: In this step, the elements of a particular level are compared pair-wise. The comparison of any two criteria w_i and w_j with respect to the goal is made using the questions of the type: of the two criteria w_i and w_j which is more important and how much. Saaty (1980) suggests the use of a 9-point scale to transform the verbal judgments into numerical quantities representing the values of a_{ij} . Table I lists the definition of 9-point scale. The judgment matrix, denoted as A , will be formed using the comparison.

$$A = [a_{ij}] = \begin{bmatrix} a_1/a_1 & a_1/a_2 & \dots & a_1/a_n \\ a_2/a_1 & a_2/a_2 & \dots & a_2/a_n \\ \dots & \dots & \dots & \dots \\ a_n/a_1 & a_n/a_2 & \dots & a_n/a_n \end{bmatrix} \quad (18)$$

2) *Calculate the Eigenvalue and Eigenvector*: Having recorded the numerical judgments a_{ij} in the matrix A , the numerical weights (w_1, w_2, \dots, w_n) can be recovered from this matrix. Then, it follows

$$y = f(y_1, y_2, y_3, y_4) = w_1 y_1 + w_2 y_2 + w_3 y_3 + w_4 y_4 \quad (19)$$

Where, w_1, w_2, w_3 and w_4 are the corresponding weights to $y_1,$

$y_2, y_3,$ and y_4 respectively, which satisfy the relation $w_1 + w_2 + w_3 + w_4 = 1$, y is the first grade index, the yield of soft capsule.

By this means, we get the weights w_1, w_2, w_3 and w_4 are 0.2507, 0.1575, 0.4884, and 0.1034 respectively.

C. Process Parameters Optimization Algorithm Design and Implementation

In the previous section of this article, the soft-sensor models of the quality indicators y_1, y_2, y_3 and y_4 have been established based on LSSVM. A linear weighted sum method is used to transform the multi-objective optimization model into a single objective optimization model. PSO algorithm is used for the single objective optimization of y .

The optimization problem can be described as follows:
Search the vector

$$x^* = [x_1^*, x_2^*, x_3^*, x_4^*]^T,$$

in the input parameters space S , which makes

$$y^* = f(x^*) = \max_{x \in S} (f(x)) \cdot \sqrt{a^2 + b^2} \quad (20)$$

Where, $S = \{[x_1, x_2, \dots, x_4]^T, x_i \in [0, 1], i = 1, 2, \dots, 4\}$.

The PSO [14] algorithm process was developed based on Matlab7.6 for the optimization of the model. The size of the swarm was set equal to 100, and the PSO algorithm ran for 50 iterations. For the PSO parameters were used: $c_1 = c_2 = 1.8$; w was gradually decreased from 1.0 towards 0.4.

The purpose of optimization is to find the input parameter values, which make the product yield y reach the largest. So $1-y$ was chosen as the fitness function, which means the smaller $1-y$, the higher the yield y , and the better the corresponding process parameters.

One of the evolutionary trajectory curves is shown as Fig.5. The change of optimizing y is represented by a thick solid line, and the average y is represented by a dashed line in Fig.5. It can be seen from the figure, the optimizing result can be reached after about 47 iterations. Its convergence rate is relatively fast. The optimizing values obtained in table II.

The best process parameter values and the yield can be obtained by doing max-min inverse transform. The corresponding theoretical value of the optimizing yield can reach 97.43%, better than the actual 93.0% average yield.

IV. DISCUSSION

The optimizing control of the soft capsule pills quality is a multi-level and multi-objective optimization problem. Yield of the product is the first grade index, and spherical degree, tailed degree, breaking pill rate, and collodion silk degree are

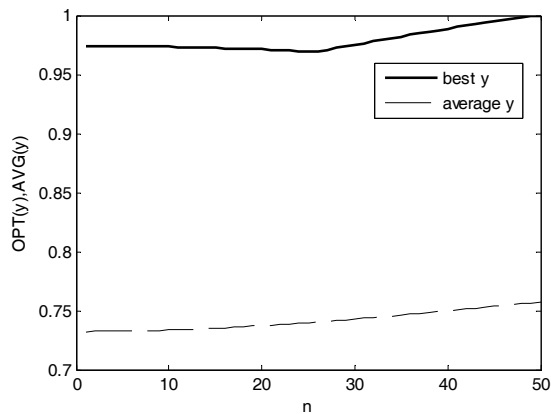


Fig.5. The evolutionary trajectory curves of the yield

secondary indexes, which are all determined by the process parameters gelatin solution viscosity, gelatin solution temperature, paraffin oil temperature and pulse pressure. The process parameters setting points should be comprehensively considered in the course of dropping pills, with the ultimate goal is to achieve maximum yield.

This paper built the LSSVM model of soft capsule dropping pills based on data-driven method. The AHP was used to determine the weights of the secondary indexes. On this basis, PSO algorithm was used to optimize the input process parameters, whose ultimate goal is to improve the yield of soft capsule pills.

Due to the limitation of the production line conditions, the system can not reach the setting points of process parameters accurately. For example, the gelatin solution viscosity is very difficult to be controlled precisely. But it can be as close as possible to the optimization values of process parameters. Meanwhile, limited by the accuracy of modeling, the yield has not yet reached the desired value, compared to preliminary statistics by using the optimized parameter values, the average yield increase about 2.7 percentage points.

V. CONCLUSION

In this paper, soft capsule pills product quality modeling and optimizing control of process parameters are discussed based on LSSVM and PSO algorithm. The mapping model between process parameters and product quality of soft capsule dropping pills was presented based on LSSVM. On this basis, PSO algorithm was used to optimize the input process parameters. The yield can increase about 2.7 percentage points by using of the optimized process parameters for production, which indicating that the method of using LSSVM and PSO in product

TABLE II
OPTIMIZED PARAMETER VALUES

Process Parameter Items	Process Parameter Values
gelatin solution viscosity x_1	0.4504
gelatin solution temperature x_2	0.5349
paraffin oil temperature x_3	0.2835
pulse pressure x_4	0.8951
fitness 1 - y	0.0257
yield y	0.9743

quality modeling and optimization of soft capsule dropping pills

is reasonable. It provides a new way for soft capsules process optimization.

REFERENCES

- [1] B. W. Wan, *Industry Large Scale System Optimization and Product Quality Control*. Beijing: Science Press, 2003. pp 1-20.
- [2] B. W. Wan, "Product quality model and quality control model for industries and their applications," *Acta Automatica Sinica*, vol. 28, pp. 1019-1024, Nov., 2002.
- [3] W. H. Wan, B. W. Wan, J. Y. Yang, "Study of neural network quality models and steady-state optimizing control for nickel flash smelting furnace," *Acta Automatica Sinica*, vol. 25, pp. 800-803, Nov., 1999.
- [4] Hadiyanto, D. C. Esveld, R. M. Boom, et al. "Product quality driven design of bakery operations using dynamic optimization". *Journal of Food Engineering*, vol. 86, pp. 399-413. 2008
- [5] Y. C. Zhang, "Product quality modeling and control based on vision inspection with an application to baking processes," Ph.D. dissertation, Dept. Elect. Eng., Georgia Institute of Technology, Cambridge, Ph.D., 2005.
- [6] Y. F. Zhang, X. L. Shao, and J. J. Lei. "Modeling and optimization of Chinese material medica pillule manufacturing process based on neural network and genetic algorithm." *Computer Engineering and Applications*, vol. 2, pp. 191-193, 216, Feb. 2005.
- [7] Y. Q. Peng, "Design of automatic control system in new automatic pulse pill dropping machine," *Pharmaceutical Engineering Design*, vol. 23, pp. 40-43, Oct. 2002.
- [8] Suykens, Vandewalle. "Recurrent least squares support vector machines". *IEEE Transactions on Circuits and Systems*, vol. 47, pp. 1109-1114, July 2000.
- [9] B. Y. Sun, D. S. Huang, "Lidar signal denoising using least-squares support vector machine". *IEEE Signal Processing Letters*, vol. 12, pp101-104, Feb. 2005.
- [10] Y. H. Wang, D. X. Huang, D. J. Gao, et al. "Nonlinear predictive control based on LS-SVM," *Control and Decision*, vol. 19, pp. 383-387, April 2004.
- [11] H. N. Rong, G. X. Zhang, W. D. Jin. "Selection of Kernel Functions and Parameters for Support Vector Machines in System Identification," *Journal of System Simulation*, vol. 18, pp. 3204-3208, Nov. 2006.
- [12] K. E. Parsopoulos, M. N. Vrahatis, "Particle swarm optimization method in multiobjective problems. *Proc of the 2002 ACM Symposium on Applied Computing*. New York, 2002: 603-607.
- [13] C. W. Chang, C. R. Wu, C. T. Lin, et al. "An application of AHP and sensitivity analysis for selecting the best slicing machine," *Computers & Industrial Engineering* (2007), doi:10.1016/j.cie. 2006. 11.006.
- [14] J. C. Zeng, J. Jie, Z. H. Cui, *Particle Swarm Optimization*, Beijing: Science Press, 2004, pp. 140-145.