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An Optimal Method of Mixed Batch Blending and Application in Traditional Chinese Medicine Blending

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Abstract: When manufacturing natural products such as medicine, oil, drink, etc, we need to mix multiple batches of natural products to ensure that the content of each component meets the requirements, i.e., the calculation of optimal blending scheme is a key to guarantee the quality of products. Manual calculation of the ratio of each batch of natural products is time consuming and inaccurate. Nowadays, this work is replaced by automatic computation of computer. This article introduced a kind of optimal all-purpose method for mixed batch blending of natural products which is fully automatic, accurate, stable and repeatable compared with previous work. Firstly, we suggested a kind of improved Gaussian Elimination Method to figure out the range of solutions. Secondly, we utilized backtrace algorithm to search the best solution in candidate solution set. Thirdly, we proposed a kind of automatic combination method to figure out solution, so that we can avoid selecting the concrete batches of the natural products. Fourthly, we evaluated all the solutions and found the optimal one according to the blending goals. To verify the validity of our method, we compared our method with genetic algorithm using the data of traditional Chinese medicine under the same conditions. The experiment results show that our method is more accurate than genetic algorithm and our method is stable during multiple tests.

Key words: Mixed batch blending method, gaussian elimination method, traditional chinese medicine blending, backtrace algorithm

INTRODUCTION

Mixed batch blending is a common method which widely exists in product processing of foods, medicine, drinks, wine, oil and flavor and there are wide requirements of it. The problem of blending is a tough technical problem. Solving of this problem can bring good fame and create large benefits for related enterprises.

Manual calculation of blending scheme is not only time consuming but also inaccurate. And now it is gradually replaced by computerized blending methods. To solve the problem of blending is to solve the problem of optimization. The common methods are linear programming(such as simplex method and Karmarkar method, etc), nonlinear programming(such as penalty function method, quadratic programming method, gradual quadratic programming method, etc.) and some intelligent method(such as genetic algorithm, simulated annealing, etc.). Liu *et al*. (2006) adopted nonlinear least square method to solve the problem of mixed batch blending of Chinese medicine extractive and realized the codes in MATLAB. Qu *et al*. (2006) took similarity degree of finger print of Chinese medicine and RDC of index components as indexes of quality evaluation, built optimal model and adopted gradual quadratic programming method to realize the mixed batch blending of Chinese medicine. Yang *et al*. (2009) selected the similarity degree of finger print and root-mean-square error of contents of index components as common optimal goal, utilized genetic algorithm to calculate coefficient of blending and made mixed batch blending of each batch of extractive. Yang *et al*. (2007) and Yang and Wang (2010) suggested a kind of method which utilized HPLC finger print to measure multiple contents of index components and utilized linear and nonlinear optimal theory to blend Chinese medicine in order to ensure the stability of multiple contents of index components of Chinese medicine mixture.

Nowadays, most of the blending methods are based on single mode of blending and some methods need to adjust the parameters in blending mathematical model when the batches of blending and the number of components change, so that it is inconvenient to use. In addition, some methods can only get partial optimum result or approximate optimum result and the calculation

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of result is unstable, such as genetic algorithm and simulated annealing algorithm. Based on the considerations above, this article suggested a kind of global optimal, accurate, stable and repeatable mixed batch blending method.

OPTIMAL MIXED BATCH BLENDING METHOD

Requirement analysis: In natural product processing, to find the optimal blending ratio of guarantee of stability of contents is a key to ensure the quality of products. After optimization, the blending ratio should basically conform to ideal blending ratio, or we can take cost into consideration to minimize the total cost. So the mixed batch blending of natural products is naturally a kind of multiple variable optimum problem under a certain constraints.

Blending method: The basic working flow of this method is shown as following:

Step 1: Before calculating the best blending ratio, we need to utilize some measurement devices to measure the contents of each component of each raw material

Step 2: Then, the computer reads the data of contents of components of each raw material into computer memory

Step 3: Set needed and related parameters, including blending goal, maximal blending error rate and blending mode, or accept default blending parameters

Step 4: Adopt automatic combination algorithm to make groups of raw material, i.e., produce the combination of offline batches and then execute step 5-7 repetitively for each combination scheme

Step 5: Utilize improved Gaussian elimination algorithm to figure out the inequality set in order to get the solution range, i.e., the range of blending ratio

Step 6: Then, utilize backtrace algorithm to search optimal solution in the range of solution, i.e., the optimal blending scheme

Step 7: Store the optimal blending scheme to blending scheme matrix

Step 8: Evaluate all blending schemes according to blending goal and produce best scheme. The blending goal may be a minimum of average deviation as Eq. 1 shows:

$$AvgDev = \frac{\sum_{i=1}^{n} \left| x_i - x_i^d \right|}{n} \tag{1}$$

Herein, AvgDev is average deviation, n is the number of components, x_i is best ratio of No. i component, x_i^d is the ideal ratio of No. i component

Step 9: In the end, produced best scheme can be used to supervise the producing of raw material, or be taken as basis of blending devices to make blending

In the method above, the key step is step 5(improved Gaussian elimination algorithm). From now on, we will discuss the improved Gaussian elimination algorithm in detail.

THE PRINCIPLE OF IMPROVED GAUSSIAN ELIMINATION ALGORITHM

Function of improved Gaussian elimination algorithm: For each scheme of offline batches, we adopt a kind of improved Gaussian elimination algorithm to solve the problem. Traditional Gaussian elimination algorithm (Li *et al*., 1982) can figure out the problem of n-linear equation set. In this article, we extended and improved the traditional method and make it figure out the n-linear inequality set. This method is different from the early method, such as linear programming and quadratic programming and this one can figure out the range of solution but not the single solution.

Mathematic model: Mathematic model of blending problem can use the following equation set to express. Eq. 3 is the symbolic expression of Eq. 2:

$$\begin{bmatrix} 1 & 1 & \cdots 1 \\ a_{10} & a_{11} & \cdots a_{1,n-1} \\ a_{20} & a_{21} & \cdots a_{2,n-1} \\ \cdots & & \\ a_{m0} & a_{m1} & \cdots a_{m,n-1} \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_{n-1} \end{bmatrix} = \begin{bmatrix} 1 \\ b_1 \\ \vdots \\ b_m \end{bmatrix} \tag{2}$$

$$AX = B \tag{3}$$

Herein, n is the total batch number, m is the total component number, A is the matrix of contents of components, X is the solution vector and B is the goal vector of blending. The solution to blending problem is to figure out the solution vector X which is nearly closest to goal vector of blending. But generally speaking, we can not get the solution vector X which confirms to goal vector of blending B. That's to say, the element b_i in blending vector B is a value where there is a certain deviation between X and B. So we convert blending problem into solving the problem of inequality set. The inequality set is shown below:

$$\begin{bmatrix} 1 \\ b_1 - c_1 \\ \vdots \\ b_m - c_m \end{bmatrix} \le \begin{bmatrix} 1 & 1 & \cdots 1 \\ a_{10} & a_{11} & \cdots a_{1,n-1} \\ a_{20} & a_{21} & \cdots a_{2,n-1} \\ \cdots \\ a_{m0} & a_{m1} & \cdots a_{m,n-1} \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_{n-1} \end{bmatrix} \le \begin{bmatrix} 1 \\ b_1 + c_1 \\ \vdots \\ b_m + c_m \end{bmatrix} \quad (4)$$

Herein, c_i is the permitted maximum deviation of No. i component and $c_i>0$. To figure out the solution range of the inequality set above, we convert inequality Eq. 4 into Eq. 2 to describe the problem, i.e., $b_i \in [b_i-c_i, b_i+c_i]$.

Solving method: Firstly, we extends the mathematic model of Gaussian elimination and multiply coefficient matrix B' on left side of B. B' is shown below:

$$B' = \begin{bmatrix} 1 & 0 & 0 \cdots 0 \\ 0 & 1 & 0 \cdots 0 \\ 0 & 0 & 1 \cdots 0 \\ \cdots \\ 0 & 0 & 0 \cdots 1 \end{bmatrix} \quad (5)$$

Then:

$$b_i = \sum_{j=0}^{m} b_j b'_{ij}$$

i.e., B = B'B. Furthermore, it is different from traditional method that we make synchronous rank transforms to matrix A and coefficient matrix B', i.e., multiplying No. i row of matrix A and matrix B' with:

$$-\frac{a_{ji}}{a_{ii}}$$

(herein, j>i) and adding No. i row to No. j row in order to eliminate the elements below principal diagonal. This procedure can use the following equations to express:

$$a_{jk} = \left(-\frac{a_{ji}}{a_{ii}}\right) \times a_{ik} + a_{jk} \quad (6)$$

$$b'_{jk} = \left(-\frac{a_{ji}}{a_{ii}}\right) \times b'_{ik} + b'_{jk} \quad (7)$$

Herein, j>i and $k \in [i, n-1]$. Similarly, we can use the similar method to eliminate the elements above principal diagonal of A. Due to matrix A and matrix B' are all coefficient matrixes and the transforms to matrix A and matrix B are synchronous, the equation AX = B'B is still correct after the transformations. The forms of matrix A and matrix B' are shown below:

$$A = \begin{bmatrix} a'_{00} & 0 & 0 \cdots 0 \\ 0 & a'_{11} & 0 \cdots 0 \\ 0 & 0 & a'_{22} \cdots 0 \\ \cdots \\ 0 & 0 & 0 \cdots a'_{mm} \end{bmatrix} \quad (8)$$

$$B' = \begin{bmatrix} b'_{00} & b'_{01} & b'_{02} \cdots b'_{0m} \\ b'_{10} & b'_{11} & b'_{12} \cdots b'_{1m} \\ b'_{20} & b'_{21} & b'_{22} \cdots b'_{2m} \\ \cdots \\ b'_{m0} & b'_{m1} & b'_{m2} \cdots b'_{mm} \end{bmatrix} \quad (9)$$

Then:

$$\max\{x_i\} = \max\left\{\frac{\sum_{j=0}^{m} b_j b'_{ij}}{a'_{ii}}\right\} \quad (10)$$

$$\min\{x_i\} = \min\left\{\frac{\sum_{j=0}^{m} b_j b'_{ij}}{a'_{ii}}\right\} \quad (11)$$

The results of 2 equations above can be figured out through analyzing monotonicity of x_i changing with b_j. And we can get the range of x_i as $[\min(x_i), \max(x_i)]$, i.e., the range of solution vector X. During the calculating procedure above, assume m+1 = n and m>0. When m+1<n or m+1>n, we can extend this method to these two situations. The principle of the method is similar, we will not repeat again.

EXPERIMENT RESULTS AND ANALYSIS

Meaning of this practical research: During past thousands of years, traditional Chinese medicine has been a treasure of Chinese people used to cure illness and build bodies. The stability of contents of components of Chinese medicine is a main requirement in the quality control of Chinese medicine production. How to effectively monitor and control the stability of the contents of each component in the production procedure and to guarantee the quality of medicine is a stringent requirement for medicine manufacturers. Therefore, to find a kind of efficient, accurate, reliable and inexpensive blending method which can guarantee the stability of contents of components after blending is of great realistic meaning and economic value.

Experiment conditions and results: We adopted Visual C^{++} to realize the blending method and applied this method to mixed batch blending of Chinese medicine. In the experiment, we processed 5 batches Chinese medicine data, optimized the result by minimizing average deviation and set the maximum blending error ratio to 10%. To specify the advantage of our method in accuracy and stability, we compared the results of our method with those of genetic algorithm. The content data of 5 batches of Chinese medicine are shown in Table 1. The comparative results of our method and genetic algorithm are shown in Table 2.

As Table 2 show, the results of 2-batch automatic combination blending, 3-batch automatic combination blending and 4-batch automatic combination blending are close to blending goals basically and all the average deviations of 3 tests are 3.9% which are quite low.

In the comparison experiment, we adopted genetic algorithm to process the 2-batch, 3-batch and 4-batch best schemes and calculate the approximate optimal solution. Due to the randomness of genetic algorithm, we repeat the experiment 3 times for each scheme in order to know the distribution of several kinds of blending results. Firstly, as we can see from Table 2, in each calculation of blending scheme using genetic algorithm, the best blending ratios and average deviations are different from each other. This is the performance of randomness of genetic algorithm. Nevertheless, our method is stable and repeatable. Secondly, as we can see from Table 2, the average deviations of 2-batch, 3-batch and 4-batch blending using our method are lower than those of genetic algorithm. Therefore, the accuracy of our method is higher than that of genetic algorithm.

Table 1: Content data of 5-batch traditional chinese medicine

Batch No.	Content of baicalin	Content of wogonoside	Content of scutellarein	Content of wogonin
Blending goal	15.57	2.68	0.74	0.27
No. 1 batch	9.43	1.95	1.63	0.46
No. 2 batch	10.55	1.84	1.75	0.42
No. 3 batch	9.94	1.97	1.68	0.47
No. 4 batch	9.62	1.73	2.70	0.55
No. 5 batch	16.12	3.02	0.38	0.17

Table 2: Results of blending by our method and genetic algorithm

Methods	Baicalin	Wogonoside	Scutellarein	Wogonin	Batch no./blending result/average deviation
Our method					
Content after 2-batch combination blending	14.390	2.726	0.744	0.254	No.3 batch: 28%; No. 5 batch: 72%
Deviation after 2-batch combination blending	7.6%	1.7%	0.5%	5.9%	Average deviation: 3.9%
Content after 3-batch combination blending	14.349	2.724	0.740	0.253	No. 1 batch: 8%; No. 3 batch: 20%; No. 5 batch: 72%
Deviation after 3-batch combination blending	7.8%	1.7%	0.0%	6.2%	Average deviation: 3.9%
Content after 4-batch combination blending	14.349	2.724	0.740	0.253	No.1 batch: 8%; No. 3 batch: 20%; No. 4 batch: 0%; No. 5 batch: 72%
Deviation after 4-batch combination blending	7.8%	1.7%	0.0%	6.2%	Average deviation: 3.9%
Genetic algorithm					
Content after No.1 2-batch blending	14.611	2.764	0.697	0.243	No. 3 batch: 24.4%; No. 5: 75.6%
Deviation after No.1 2-batch blending	6.2%	3.1%	5.8%	9.9%	Average deviation: 6.2%
Content after No.2 2-batch blending	14.51	2.747	0.718	0.248	No. 3 batch: 26%; No. 5 batch: 74%
Deviation after No.2 2-batch blending	6.8%	2.5%	3.0%	8.2%	Average deviation: 5.1%
Content after No.3 2-batch blending	13.78	2.623	0.871	0.283	No. 3 batch: 37.8%; No. 5 batch: 62.2%
Deviation after No.3 2-batch blending	11.5%	2.1%	17.8%	5.0%	Average deviation: 9.1%
Content after No.1 3-batch blending	13.837	2.638	0.847	0.278	No. 1 batch: 8.7%; No. 3 batch: 27.5%; No. 5 batch: 63.8%
Deviation after No.1 3-batch blending	11.1%	1.6%	14.4%	2.9%	Average deviation: 7.5%
Content after No.2 3-batch blending	13.781	2.629	0.856	0.280	No. 1 batch: 10.2%; No. 3 batch: 26.8%; No. 5 batch: 63.0%
Deviation after No.2 3-batch blending	11.5%	1.9%	15.7%	3.7%	Average deviation: 8.2%
Content after No.3 3-batch blending	13.696	2.626	0.848	0.278	No. 1 batch: 26.8%; No. 3 batch: 10.2%; No. 5 batch: 63%
Deviation after No.3 3-batch blending	12.0%	2.0%	14.6%	3.1%	Average deviation: 7.9%
Content after No.1 4-batch blending	14.283	2.690	0.873	0.264	No.1 batch: 8.7%; No. 3 batch: 7.1%; No. 4 batch: 12.6%; No. 5 batch: 71.6%
Deviation after No.1 4-batch blending	8.3%	0.4%	17.9%	2.1%	Average deviation: 7.2%
Content after No.2 4-batch blending	14.899	2.800	0.712	0.233	No.1 batch: 4.7%; No.3 batch: 5.5%; No. 4 batch: 8.7%; No.5 batch: 81.1%
Deviation after No.2 4-batch blending	4.3%	4.5%	3.9%	13.7%	Average deviation : 6.6%
Content after No.3 4-batch blending	14.168	2.669	0.908	0.270	No.1 batch: 11.0%; No. 3 batch: 4.7%; No. 4 batch: 14.2%; No. 5 batch: 70.1%
Deviation after No.3 4-batch blending	9.0%	0.4%	22.7%	0.02%	Average deviation: 8.0%

CONCLUSION

This article introduced a kind of all-purpose mixed batch blending method. We suggested a kind of improved Gaussian elimination algorithm to figure out the range of solution. Besides, we utilized automatic combination algorithm to calculate the best blending scheme so that we can avoid selecting the concrete batches manually. In the experiment, we utilized our method and genetic algorithm to calculate the best schemes of 2-batch blending, 3-batch blending and 4-batch blending and our method achieved better results. The comparison experiment results show that the accuracy of our method is higher than that of genetic algorithm and our method is stable and repeatable.

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