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An Improved Sequential Quadratic Programming Method Based on Positive Constraint Sets

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SQP (sequential quadratic programming) is an effective method to solve nonlinear constraint problems, widely used in chemical process simulation optimization. At present, most optimization methods in general chemical process simulation software have the problems of slow calculation and poor convergence. To solve these problems, an improved SQP optimization method based on positive constraint sets was developed. The new optimization method was used in the general chemical process simulation software named optimization engineers, adopting the traditional Armijo type step rule, L-BFGS (Limited-Memory BFGS) algorithm and rules of positive definite matrix. Compared to the traditional SQP method, the SQP optimization method based on positive constraint sets simplifies the constraint number of corresponding subproblems. L-BFGS algorithm and rules of positive definite matrix simplify the solution of the second derivative matrix, and reduce the amount of storage in the calculation process. The new optimization method saves the computer memory, and makes the optimal calculation easier to converge, using precise penalty function and step rule. The example shows that the optimization function of optimization engineers based on the improved SQP optimization method can meet the needs of chemical process optimization calculation. The iteration times can be reduced by about 10 %, and the calculation time can be reduced by 5.3 %. It is suitable for the simulation optimization calculation of general chemical process.

1. Introduction

The current chemical production scale is getting larger and more and more automated, chemical production needs to pursue higher economic efficiency under the conditions of environmental protection and efficient use of energy, and there is an urgent need to optimize the calculation of large-scale chemical simulation software. Although existing large-scale simulation software, such as Aspen Plus, provides powerful modeling functions for chemical process, the purpose of simulation is not to simulate the province, but more importantly to analyze and optimize. Aspen Plus uses SQP as the default algorithm for optimization, which is a fast and efficient method for solving the Nonlinear programming problem, Biegler applied SQP method to process optimization in modular environment, developed infeasible path method (Biegler and Cuthrell, 1985a), feasible path method (Biegler and Hughes, 1985b) and hybrid algorithm.

The traditional SQP method still faces the problem that every step of the quadratic programming subproblem must have a solution in the iterative process, because the constraint condition of the subproblem is linear approximation of the constraint condition of the original problem, the constraint region may be empty, which can not guarantee the correctness of the calculation. Based on the above, Liu et al. (2015) established a modular relaxation SQP feasible direction algorithm for solving inequality constrained problems, which reduced the problem of sub-incompatibility, Hespanhol and Quirynen (2019) established an SQP algorithm based on block-wise quasi-Newton Jacobian updates for nonlinear optimal control, Wang et al. (2019) proposed the mode relaxation SQP algorithm with the help of the mode relaxation method and the sequence linear equation set, and the numerical calculation is good, but it is difficult to integrate with the chemical

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process, Yue et al. (2009) introduced the concept of filter-SQP into chemical process optimization under modular environment, a step-by-step normalization strategy is proposed to develop a suitable chemical optimization system, but each iteration requires updating the filter set, which requires more computation and storage space. Johannes et al. (2019) proposed two L-BFGS trust-region methods for large-scale optimization with linear equality constraints, these algorithms are more efficient at solving the problem of computer memory usage, although the methods are better suited to the linear equation constraint problem.

In order to solve the problem of sub-problem compatibility of traditional SQP method and the problem of excessive computation volume and storage space required for computation of neutron problems, inspired by the idea of die relaxation and stepwise specification strategy proposed by other scholars, the Optimization Engineer platform of general chemical process simulation and optimization software is programmed using C++ code, the SQP method of active constraint set, the traditional Armijo-type step rule and the L-BFGS algorithm and stepwise specification strategy applicable to the actual chemical calculation, to develop the optimization calculation function applicable to general chemical process. Compared with the previous SQP method, the new algorithm is more suitable for chemical simulation calculations and can greatly reduce the calculation time while ensuring convergence accuracy.

2. SQP algorithm based on improved positive constraint sets

2.1 Preliminary treatment

The optimization problem of large-scale chemical process is nonlinear, and it is a nonlinear optimization problem with equality and inequality constraints:

$$\begin{aligned} \min. \quad & f(x) \\ s.t. \quad & g_i(x) = 0, i \in K = \{1,...,m_e\} \\ & g_i(x) \le 0, i \in J = \{m_e+1,...,m\} \end{aligned} \tag{1}$$

$x \in R^n$, f, g_i are all quadratic continuous differentiable. The Lagrangian:

$$L(x,u) = f(x) + \sum_{i=1}^{m} u_i g_i(x) \tag{2}$$

Where $u=(u_1,...u_m) \in R^m$ is a general constrained Lagrange multiplier vector in Eq(1). SQP is a method that transforms the nonlinear programming problem into a series of quadratic programming problems. For the above problems, the solutions are equivalent to the following quadratic programming problems:

$$\begin{aligned} \min. \quad & \frac{1}{2} d^T B d + \nabla f(x)^T d \\ s.t. \quad & \nabla g_i(x)^T d + g_i(x) = 0, i \in K \\ & \nabla g_i(x)^T d + g_i(x) \le 0, i \in J \end{aligned} \tag{3}$$

Solving the above formula and getting the step size d_k.

2.2 Active set method

There are active set method (Babonneau and Vial, 2009), dual method (Kudela et al., 2017) and interior point method (Yang, 2014) to solve quadratic programming problems. The positive set method considers that the non-positive inequality constraint has no effect near the solution, while the active inequality constraint can be replaced by the equality constraint because it is zero at the solution (Liu and Ma, 2018), so it is a feasible point method, every iteration only needs to solve equality constraint, so the active set method is used to solve quadratic programming problem in this software.

Let $I_k = \{i \in I_0^k \cup J \mid g_i(x_k) + \nabla g_i(x_k)^T d = 0\}$, $I_0^k = \{i \in K \mid g_i(x_k) + \nabla g_i(x_k)^T d = 0\}$, and $N_k = N_{I_k}(x^k)$, Then d_k is calculated by the followong formula:

$$d_k = \begin{cases} d_k^0 & N_k^T N_k = 0 \\ d_k^0 - Q_k^T (\|d_k^0\|^r e^k + g^k) & N_k^T N_k \ne 0 \end{cases} \tag{4}$$

e^k is identity matrix, $g_k = g_i(x^k + d_k^0)$, $i \in I_k$.

2.3 Using L-BFGS to replace Hessian matrix

For the second derivative matrix used in the solution, the finite difference method is usually used to approximate the value of the function corresponding to the discrete values of the variables. The principle is that the stationary point is obtained by the Newton method. In essence, the second derivative is obtained by using the second order Taylor series:

$$f''(x_i) = (\frac{\partial^2 f}{\partial x^2}) \approx \frac{f(x_i+\sigma)+f(x_i-\sigma)-2f(x_i)}{\sigma^2} \tag{5}$$

Using Eq(5) to solve the Hessian matrix requires a large number of iterative solutions, which is not only complicated but also takes up a large amount of computer memory and is not suitable for computer programming, Fletcher (1987) proposed BFGS algorithm for the approximate matrix B_K of L (x,u) Hessian matrix.In the first step, B_K is considered as a unit matrix:

Let $s_k = x_{k+1} - x_k$, $y_k = \nabla_x L(x_{k+1}, u_{k+1}) - \nabla_x L(x_k, u_{k+1})$, BFGS correction formula requires s_k and y_k to satisfy the curvature condition, so Powell proposed a vector y_k correction formula to satisfy the above conditions, let $z_k = \theta_k y_k + (1-\theta_k) B_k s_k$,

$$\theta_k = \begin{cases} 1, & 若 s_k^T y_k \geq 0.2 s_k^T B_k s_k \\ \dfrac{0.8 s_k^T B_k s_k}{s_k^T B_k s_k - s_k^T y_k}, & 若 s_k^T y_k < 0.2 s_k^T B_k s_k \end{cases} \tag{6}$$

The constrained BFGS correction formula of matrix B_k is:

$$B_{k+1} = B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \frac{z_k z_k^T}{s_k^T z_k} \tag{7}$$

Although the BFGS algorithm iteratively approximates the Hessian matrix, a large number of B_k matrices are stored during the computation, usually the B_k matrix being the sparse matrix. The computer memory required to store the B_k matrix is about 7 GB, which increases the computation time in 10,000 dimensions, plus the overall storage space required for the optimization algorithm. In order to solve the above problems, the L-BFGS algorithm (Shen et al., 2020) is used to solve the problems of storage and computing speed. Instead of storing all the s_K and y_k matrices separately, the target matrix B_k is calculated by using all the s_k and y_k matrices, and the front s_k and y_k can be discarded when the target storage is reached, to save computer memory and computing time by discarding finite precision.

2.4 Linear search

In order to ensure convergence, the search step is usually determined by value function.

$$P_\sigma(x) = f(x) + \frac{1}{\sigma}[\sum_{i\in K} |g_i(x)| + \sum_{i\in J} |[\max\{0, -g_i(x)\}]|] \tag{8}$$

The penalty parameter $\sigma > 0$. And combined with the Armijo criterion, the line search speed and accuracy: $\beta \in (0,1)$, $\sigma \in (0,0.5)$, the step size factor $\alpha_k = \beta^{m_k}$, m_k is the smallest nonnegative integer to achieve the following inequality:

$$f(x_k + \beta^m d_k) \leq f(x_k) + \sigma\beta^m \nabla f(x_k)^T d_k \tag{9}$$

Combining them,seeking d_k, is the following:

$$P_\sigma(x_k + \alpha_k d_k) \leq \min_{\alpha\in(0,\delta]} P_\sigma(x_k + \alpha d_k) + \eta_k \tag{10}$$

among them $m_k := m$, $x_{k+1} := x_k + \beta^{m_k} d_k$.

2.5 Chemical simulation optimization combined with the algorithm

The algorithm is combined with the optimization of chemical engineering simulation. The calculation steps are as follows:

1) Obtain the object function and constraint function of user input;
2) The objective function and the constraint function are calculated by using the general chemical process simulation and optimization software;
3) Obtain gradient, given the initial unit matrix B_K;

4) d_k is obtained by solving subproblem Eq(3) with positive set method;
5) The calculation is converged and the result is output; otherwise, proceed to the next step;
6) Use $\ell 1$ value function and Armijo criterion;
7) Let k: = k + 1 and continue to step 3).

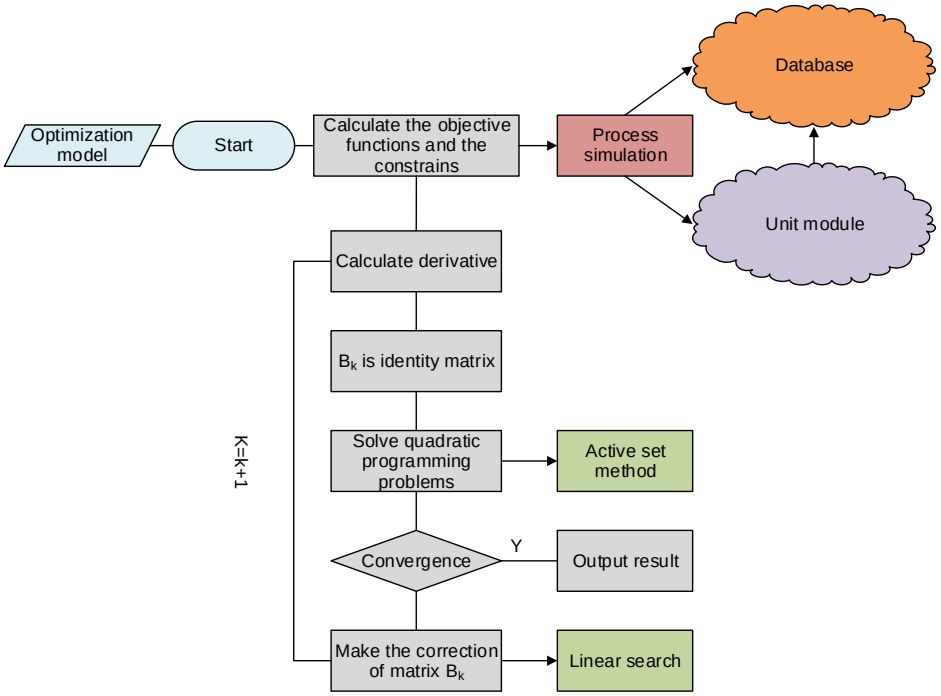

Figure 1: Schematic diagram of chemical engineering optimization calculation process

3. Case study

3.1 Flashing process optimization

Figure 2 shows the gas separation unit, it mainly separates the liquefied gas from the catalytic unit into high-purity propylene, propane and alkylated materials by distillation, and the by-products are ethane and carbon tetra liquefied gas. A four-tower conventional separation process is usually used.

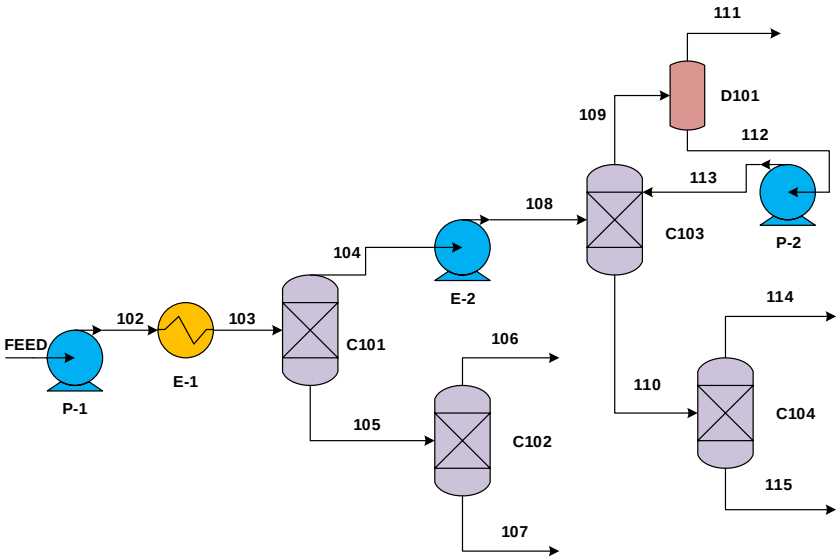

Figure 2: Schematic diagram of benzene-toluene flash evaporation process

In the process, the temperature of Feed is T_1 = 35 ℃, the pressure p_1 = 1.5 Mpa, feed mass flow F_1 = 59,541 kg/h, the temperature of E101 is T_2 = 65 ℃, reflux ratio of C104 is R = 22, flash pressure of D101 is p_2 = 2.5 Mpa, the purpose of the optimization is to maximize the Propane yield f(x) in the C101 tower bottom product by adjusting the reflux ratio of C101, the heating temperature of E-1, and the flash evaporation pressure of D101.

From the above description, the following model is constructed:

$$\begin{aligned} &Max \quad f(x) = F_{115}.C_{c3} \\ &s.t. \quad 0 < C_{c3} < 1 \\ &\quad 15 \le R \le 30 \\ &\quad 50 < T_2 < 100 \\ &\quad 1.5 < p_2 < 3 \end{aligned} \tag{11}$$

F_{115}——flow of streams 115;
C_{C3}——Molar fraction of Propane in stream 115;

3.2 Discussion of results

In the general chemical process simulation optimization software, the traditional SQP method, the trust region SQP method, and the improved active constraint set SQP method are used to optimize the above processes. The results are shown in Table 1.

Table 1: Comparison of the results of the three optimization methods

	Traditional SQP method	Filter-SQP method	Improved active constraint set SQP method
T_2/℃	67.00	66.45	66.53
F_{115}/kg·h^{-1}	5,722.12	5,723.21	5,723.03
p_2/MPa	2.48	2.49	2.49
R	26	26	26
f(x)/ kg·h^{-1}	5,693.51	5,694.59	5,694.41
Number of iterations	31	30	26
calculating time/s	109.91	106.67	101.32

The comparison results show that the three methods can converge and the results are almost the same, which shows that the three methods can be used in chemical engineering simulation optimization. Compared with the traditional SQP method, the Filter-SQP method can reduce he number of iterations by about 3.23 %, and the improved active set SQP method can reduce by about 6.45 %, the Filter-SQP method can save about 2.95 % computation time, the improved active set SQP method saves about 7.81 % of the computation time, and can be roughly viewed by the computer's memory usage. Under the same running conditions, the improved active set SQP method has lower memory usage than the former two methods, the main reasons are as follows: first, the improved active set SQP method uses the L-BFGS algorithm in machine learning. Compared with the BFGS algorithm, although the principle is similar, the L-BFGS algorithm has obvious advantages in the matrix storage, secondly, the active set method is a feasible point method, which avoids unnecessary computation and iterative search.

4. Conclusion

An improved SQP optimization algorithm was developed by combining the active set SQP method with the L-BFGS algorithm of machine learning, using Armijo's step length law, on a general-purpose chemical process simulation software optimization engineer platform, combined with the process simulation function of the software. Examples show that the algorithm can reduce the number of iterations by about 5 % and save 7-8 % of computation time compared to the traditional SQP method. The algorithm also has some limitations, the algorithm implementation is combined with chemical simulation, there is no corresponding development and example testing in other fields, the applicability in different fields is not clear. The step size determination in the algorithm is relatively traditional and simple, in order to make the algorithm more general and accurate, step size search strategies such as arc search with specificity and uniqueness are not adopted, and many advanced step size search strategies need to be studied and improved in the future to improve the stability of the algorithm and accelerate the convergence of the algorithm.

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