Simulated annealing[1] , which was inspired by the natural process of annealing solids. The physical process of annealing involves slowing cooling metal, so it adopts a low energy, crystalline state. When the temperature of the metal is high, the particles within the metal are active, changing the metal structure. As the temperature is lowered, the particles are limited in movement since a high energy cost are very limited to configurations with a lower energy. Simulated annealing uses the idea of a physical process, in a computational model. The basic algorithm maintains both a state and a temperature, which is initially high and is reduced to near zero according to a cooling schedule. The configuration is typically a solution to the optimization, and at each iteration of the algorithm, this solution is changed to produce a new solution. The quality of the solution is evaluated using the objective function, and a new state is selected from the two solutions. When a new solution is better than the previous, the new solution is chosen, but when the new solution has a lower quality than the existing solution, it may be accepted with a probability depended on the current temperature and the difference in quality. With certain cooling schedules, annealing can be guaranteed to find a global minimum.

From a high temperature, this algorithm calculates the initial solution in the high temperature state, and then generates a disturbance with the preset neighborhood function, so as to obtain a new state, that is, simulate the disordered motion of particles, and compare the energy in the old and new states, that is, the solution of the objective function. If the energy of the new state is less than that of the old state, the state is transformed; If the energy of the new state is greater than that of the old state, the transformation occurs with a certain probability criterion. When the state is stable, it can be regarded as reaching the optimal solution of the current state, then it can start to cool down, continue to iterate at the next temperature, and finally reach the stable state of low temperature, and the results of simulated annealing algorithm are obtained.

0.1 state space and neighborhood function

State space is also called search space, which consists of a set of coded feasible solutions. The neighborhood function should satisfy as much as possible that the generated candidate solutions spread all over the state space. It is usually composed of the method of generating candidate solutions and the probability distribution of generating candidate solutions. Candidate solutions are generally obtained by randomly sampling the solution space according to a certain probability density function, and the probability distribution can be uniform distribution, normal distribution, exponential distribution, etc.

0.2 State transition probability (Metropolis criterion)

State transition probability refers to the probability of switching from one state to another. Metropolis criterion is generally adopted in simulated annealing algorithm, as follows:

$$P = \begin{cases} 1 & E\left(x_{\text{new}}\right) < \mathrm{E}\left(x_{\text{old}}\right) \\ \exp\left(-\frac{\mathrm{E}(x_{\text{new}})-\mathrm{E}(x_{\text{old}})}{T}\right), & \mathrm{E}\left(x_{\text{new}}\right) \geq \mathrm{E}\left(x_{\text{old}}\right) \end{cases}$$

0.3 Cooling schedule

The cooling schedule refers to the cooling function when cooling from a high-temperature state t to a low-temperature state. If the temperature at the time is $T(t)$, the cooling mode of the classical and fast simulated annealing algorithms are respectively:

$$\mathrm{T(t)} = \frac{T_0}{\lg(1+t)}$$
$$\mathrm{T(t)} = \frac{T_0}{1+t}$$

0.4 initial temperature

Generally speaking, the greater the initial temperature, the greater the probability of obtaining a high-quality solution, but the time will also increase. Therefore, the determination of the initial temperature should consider

both the calculation efficiency and the optimization quality. The commonly used methods include: (1) Uniformly sample a group of States, and take the variance of the target value of each state as the initial temperature. (2) Randomly generate a group of States, determine the maximum target value difference between the bright states, and then use a certain function to determine the initial temperature according to the difference, such as:

$$T_0 = -\frac{\Delta_{\max}}{Pr}$$

0.5 cycle termination criteria

Internal circulation termination criteria: (1) Check whether the mean value of the objective function is stable

(2) The target value of several consecutive steps changes little

(3) Sample according to a certain number of steps

External circulation termination criteria

(1) Set termination temperature

(2) Sets the number of outer loop iterations

(3) The optimal value searched by the algorithm remains unchanged for several consecutive steps

(4) Check whether the system entropy is stable

References

[1] SP Brooks and BJT Morgan. *Optimization using simulated annealing.*