Proceedings of the 5th WSEAS Int. Conf. on APPLIED INFORMATICS and COMMUNICATIONS, Malta, September 15-17, 2005 (pp296-300)

Simulated Annealing Method for Regional Analysis

JAN PANUS, STANISLAVA SIMONOVA
Institute of System Engineering and Informatics
University of Pardubice
Studentská 84, 532 10 Pardubice
CZECH REPUBLIC
http://www.upce.cz

Abstract: - Mathematical optimization is the formal title given to the branch of computational science that seeks to answer the question „What is best?“ for problems in which the quality of any answer can be expressed as a numerical value. Such problems arise in all areas of mathematics, the physical, chemical and biological sciences, engineering, architecture, economics, and management, and the range of techniques available to solve them is nearly as wide. Such problems arise also in the information sources of local authorities. The modernizing Government agenda is accelerating, with the emphasis on the local delivery of improved public service. Thus, to get a quality answer to a strategic enquiry, the special methods are necessary; when a simulated annealing method seems to be suitable.

Key-Words: Simulated Annealing Method, Optimization – Global Optimization, Regional Data Sources, Strategic Questions

1 Introduction

Regional data sources are supposed to serve for analyzing and answering strategic regional enquiries, so that this informational environment would serve for an effective area administration and also as an information resource for other institutions and for citizens. From a data analysis perspective, the local authority approach is the process of gathering meaningful information about the subject matter being researched that will help the individual(s) analyzing the information draw conclusions or make assumptions. From an information systems perspective, the local authority approach is the system that provides users with online analytical processing or data analysis to answer strategic questions and identify significant trends or patterns in the information that is being examined.

2 Regional Data Sources

Local authorities exist in a very complex organizational environment, which has been subjected to an ever increasing pace of changes. This situation has generated a huge impact on the local government's reaction towards two major elements in its administration – decision making and technology approaching. Methods for gathering high-quality and meaningful information are methods of mathematical optimization.

2.1 Requirement of Strategic Enquiries

Information systems within public administration are most frequently realized by database software. Above all, these are so-called transaction database systems, which are designed for work with operational data of the organization. Transaction systems work with actual operational data, they are, however, less suitable for analyses in time relations, more complex enquiries etc. Another approach to data sources is brought in by data warehouse technologies, when data are drawn from heterogeneous sources of transaction applications and are stored for a certain period of time, so that they can be used for comparisons, analyses and predictions [5].

Regional data warehouse can be realized on different levels of elaboration and efficiency. The simplest architecture is represented by the application of enquiry tools directly on operational data; the second is the model of local data marts, which already involves separation of enquiry mechanism from operational data and creation of subject-oriented enquiries; the third possible solution is represented by independent data marts, extended by the process of extraction and transformation of heterogeneous data; and finally, the most ideal, complicated and financially demanding is the architecture of enterprise data warehouse with dependent data marts.

The selection of a suitable variant of data warehouse architecture must reflect current needs and possibilities of regional institutions. Currently local authorities have minimal experience about data warehousing and data mining processes. Data warehouse building is complicated, and financially and organizationally demanding. The solution can be to begin with easier variants - either the application of enquiry tools directly on operational data (see Figure 1) or the model of local data marts, which already involves separation of enquiry

Proceedings of the 5th WSEAS Int. Conf. on APPLIED INFORMATICS and COMMUNICATIONS, Malta, September 15-17, 2005 (pp296-300)

mechanism from operational data and creation of subject-oriented enquiries (see Figure 2).

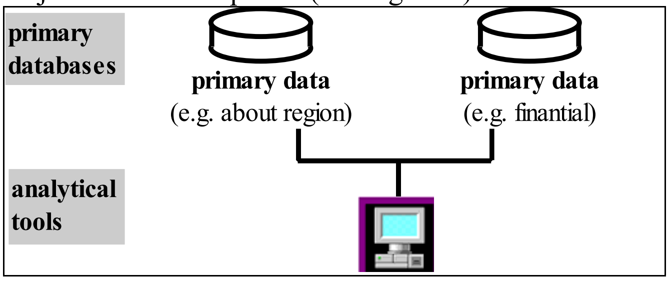

Fig. 1: Application of analytical tools directly on operational data

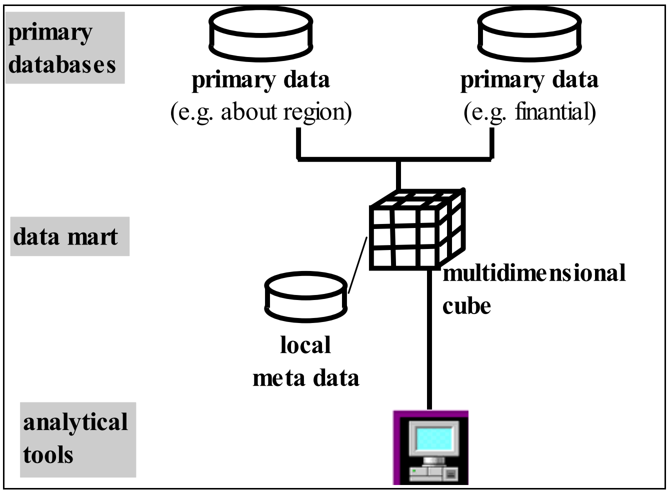

Fig. 2: Separation of enquiry mechanism from operational data

2.2 Optimization Methods

Mathematical optimization is the formal title given to the branch of computational science that seeks to answer the question „What is best?" for problems in which the quality of any answer can be expressed as a numerical value. Such problems arise in all areas of mathematics, the physical, chemical and biological sciences, engineering, architecture, economics, and management, and the range of techniques available to solve them is nearly as wide.

The goal of an optimization problem can be formulated as follows: find the combination of parameters (independent variables) which optimize a given quantity, possibly subject to some restrictions on the allowed parameter ranges. The quantity to be optimized (maximized or minimized) is termed the *objective function*; the parameters which may be changed in the quest for the optimum are called control or *decision variables*; the restrictions on allowed parameter values are known as *constraints*. A general constrained *nonlinear programming problem* (NLP) takes the following form

$$\begin{array}{lll} \textit{minimize} & f(x) & \\ \textit{subject to} & h(x) = 0 & x = (x1,\ldots, xn) \qquad (1) \\ g(x) \le 0 & & \end{array}$$

where $f(x)$ is an objective function that we want to minimize. $h(x) = [h_1(x), \ldots, h_m(x)]^T$ is a set of m equality constraints, and $g(x) = [g_1(x), \ldots, g_k(x)]^T$ is a set of k inequality constraints. All $f(x)$, $h(x)$, and $g(x)$ are either linear or nonlinear, convex or nonconvex, continuous or discontinuous, analytic (i.e., in closed-form) or procedural (i.e., evaluated by some procedure or simulation). Variable space X is composed of all possible combinations of variables x_i, $i = 1, 2, \ldots, n$. In contrast to many existing NLP theory and methods, our formulation has no requirements on convexity, differentiability, and continuity of the objective and constraint functions.

Without loss of generality, we discuss our results with respect to minimization problem (1), knowing that maximization problems can always be transformed into minimization problems by negating their objective functions. Therefore, we use optimization and minimization interchangeably in this thesis. Two special cases are involved: a) an unconstrained NLP if there is no constraint and b) a constraint-satisfaction[7] problem if there is no objective function.

With respect to minimization problem (1), we make the following assumptions.

- Objective function $f(x)$ is lower bounded, but constraints $h(x)$ and $g(x)$ can be either bounded or unbounded.
- All variables x_i ($i = 1, 2, \ldots, n$) are bounded.
- All functions $f(x)$, $h(x)$, and $g(x)$ can be either linear or nonlinear, convex or nonconvex, continuous or discontinuous, differentiable or non-differentiable.

In some applications, variables are restricted to take prespecifed values. According to the values that variable x takes, we have three classes of constrained NLPs:

- **Discrete problems**: Variable x is a vector of discrete variables, where component x_i takes discrete and finite values, such as integers. Although variable space X at this time is finite (because variable x is bounded), it is usually very huge, making it impossible to enumerate every combination of x.
- **Continuous problems**: Variable x is a vector of continuous variables, $x_i \in R$, and $x \in R^n$. Variable space X is infinite.
- **Mixed-integer problems**: Some variables take discrete values while others take continuous values. Let I_d be the set of indices of discrete variables, and I_c be those of continuous variables.

Active research in the past four decades has produced a variety of methods for solving general constrained nonlinear programming problems. They fall into one of two general formulations, direct solution or transformation-based. The former aims to directly solve constrained NLP (1) by searching its feasible regions, while the latter first transforms (1) into another form before solving it. Transformation-based formulations can be further divided into penalty-based and Lagrangian-based. For each formulation, strategies that can be applied are classified as local search, global search, and global optimization.

Local search. Local search methods use local information, such as gradients and Hessian matrices, to generate iterative points and attempt to locate *constrained local minima* (CLM) quickly. Local search methods may not guarantee to find CLM, and their solution quality is heavily dependent on starting points. These CLM are *constrained global minima* (CGM) [3] only if (1) is convex, namely, the objective function $f(x)$ is convex, every inequality constraint $g_i(x)$ is convex, and every equality constraint $h_i(x)$ is linear.

Global search. Global search methods employ local search methods to find CLM and, as they get stuck at local minima, utilize some mechanisms, such as multistart, to escape from these local minima. Hence, one can seek as many local minima as possible and pick the best one as the result. These mechanisms can be either deterministic or probabilistic and do not guarantee to find CGM.

Global optimization. Global optimization methods are methods that are able to find CGM of constrained NLPs. They can either hit a CGM during their search or converge to a CGM when they stop.

In this paper, we survey one of the existing methods for solving each class of discrete, continuous, and mixed-integer constrained NLPs. It is simulated annealing (SA), that was developed for solving unconstrained NLPs. SA searches in variable space X and it (SA) does probalistic descents in variable x space with acceptance probalistic governed by a temperature.

3 Strategic Data

Regional data sources involve huge number of data, it means there is no problem in quantity of data. But a big problem is in the area of strategic question [6]; it means it is difficult to find optimal solution for particular regional strategic processes.

More mathematical methods make possible to search optimum in problem solution. One of them is method of Simulated Annealing that finds global optimum.

3.1 Method of Simulated Annealing

As its name implies, the SA exploits an analogy between the way in which a metal cools and freezes into a minimum energy crystalline structure (the annealing process) and the search for a minimum in a more general system. We briefly overview SA and its theory [1] for solving discrete unconstrained NLPs or combinatorial optimization problems. A general unconstrained NLP is defined as

$$\textit{minimize}_i \qquad f(i) \qquad \textit{for} \qquad i \in S \tag{2}$$

```
procedure SA
  set starting point i = i0;
  set starting temperature T = T^0 and
  cooling rate 0 < α < 1;
  set N_T (number of trials per temperature);
  while stopping condition is not satisfied do
      for k ← 1 to N_T do
         generate trial point i` from S_i using q(i; i`);
         accept i` with probability A_T (i; i`)
      end for
         reduce temperature by T ← α x T;
      end while
end procedure
```

Fig. 3: Simulated annealing (SA) algorithm.

where $f(i)$ is an objective function to be minimized, and S is the *solution space* denoting the finite set of all possible solutions.

A solution i_{opt} is called a *global minimum* if it satisfies $f(i_{opt}) \leq f(i)$, for all $i \in S$. Let S_{opt} be the set of all the global minima and $f_{opt} = f(i_{opt})$ be their objective value. Neighborhood S_i of solution i is the set of discrete points j satisfying $j \in S_i, \leftrightarrow i \in S_j$.

Figure 3 shows the procedure of SA for solving unconstrained problem (2). q(i; i`), the *generation probability*, is defined as $q(i; i`) = 1/|S_i|$ for all $i` \in S_i$, and AT (i; i`), the *acceptance probability* of accepting solution point i‘, is defined by:

$$AT\,(i;\,i0) = exp\left(-\frac{\left(f(i`)-f(i)\right)^{+}}{T}\right), \tag{3}$$

where $a^+ = a$ if $a > 0$, and $a+ = 0$ otherwise.

Accordingly, SA works as follows. Given current solution i, SA first generates trial point $i`$. If $f(i`) < f(i)$, $i`$ is accepted as a starting point for the next iteration; otherwise, solution $i`$ is accepted with probability

$$exp\left(-\frac{f(i;)-f(i)}{T}\right).$$

The worse the $i`$ is, the smaller is the probability that $i`$ is accepted for the next iteration. The above procedure is repeated N_T times until temperature T is reduced.

Theoretically, if T is reduced sufficiently slowly in logarithmic scale, then SA will converge asymptotically to an optimal solution $i_{opt} \in S_{opt}$ [1]. In practice, a geometric cooling schedule, $T \leftarrow \boldsymbol{\alpha} T$, is generally utilized to have SA settle down at some solution i^* in a finite amount of time.

SA can be modeled by an inhomogeneous Markov chain that consists of a sequence of homogeneous Markov chains of finite length, each at a specific temperature in a given temperature schedule. According to generation probability $q(i;\ i`)$ and acceptance probability $A_T\ (i;\ i`)$, the one-step transition probability of the Markov chain is:

$$P_T\ (i;\ i`) = \begin{cases} q((i,i`))\,A_T(i,i`) & \text{if } i`\in S_i \\ 1-\sum_{j\in S_i, j\neq i} P_T(i,j) & \text{if } i`=i \\ 0 & \text{otherwise} \end{cases} \qquad (4)$$

and the corresponding transition matrix is

$$P_T = [P_T\ (i;\ i`)].$$

It is assumed that, by choosing neighborhood S_i properly, the Markov chain is irreducible, meaning that for each pair of solutions i and j, there is a positive probability of reaching j from i in a finite number of steps.

Consider the sequence of temperatures $\{T_k;\ k = 0, 1, 2, ...\}$, where $T_k > T_{k+1}$ and $lim_{k\to\infty} T_k = 0$, and choose N_T to be the maximum of the minimum number of steps required to reach an i_{opt} from every $j \in S$. Since the Markov is irreducible and search space S is finite, such NT always exists. The asymptotic convergence theorem of SA is stated as follows.

Theorem The Markov chain modeling SA converges asymptotically to a global minimum of S_{opt} if the sequence of temperatures satisfies:

$$Tk \geq \frac{N_T \Delta}{\log_e(k+1)}, \qquad (5)$$

where $\Delta = \max_{i,j\in S} \{f(j) - f(i) \mid j \in S_i\}$.

The proof of this theorem is based on so-called local balance equation [1], meaning that:

$$\pi_T(\,i\,)P_T(\,i,\,i`) = \pi_T(\,i`)P_T(\,i`,\,i\,), \qquad (6)$$

where $\pi_T(i)$ is the stationary probability of state i at temperature T.

Although SA works well for solving unconstrained NLPs, it cannot be used directly to solve constrained NLPs that have a set of constraints to be satisfied, in addition to minimizing the objective. The widely used strategy is to transform constrained NLP (1) into an unconstrained NLP using penalty formulations [2]. For static penalty formulation [2], it is very difficult to choose suitable penalty γ: if the penalty is too large, SA tends to find feasible solutions rather than optimal solutions. For dynamic penalty formulation [4], unconstrained problem [4] at every stage of λ(k) has to be solved optimally [1, 2] in order to have asymptotic convergence. However, this requirement is dificult to achieve in practice, given only a finite amount of time in each stage. If the result in one stage is not a global minimum, then the process cannot be guaranteed to find constrained global minima. Therefore, applying SA to a dynamic-penalty formulation does not always lead to asymptotic convergence. Besides, SA cannot be used to search in a Lagrangian space, because minimizing Lagrangian function.

For special case of (1), the generalized discrete augmented Lagrangian function is defined as

$$L_d(x,\lambda) = f(x) + \lambda^T H(h(x)) + 1/2\,\|h(x)\|^2 \qquad (7)$$

where $\lambda = \{\lambda_1, \lambda_2, ... \lambda_m\}$ is a set of Lagrange multipliers, H is a continuous transformation function that satisfies

$H(x) = 0, \leftrightarrow x = 0$, and $\|h(x)\|^2 = \sum_{i=1}^{m} h_i^2(x)$

3.2 Strategic Information

The basic principle of the method of Simulated Annealing deals with the optimum searching by help of criteria changing. This principle seems to be suitable for strategic regional decisions. The management of local authorities needs optimum solution for particular problems in the context of various regional indicators.

Example of these strategic regional questions are number of doctor's surgery in the region (see Figure 4), number of hospitals, number of primary schools in some district, size of regional high school / university (number of students) etc.

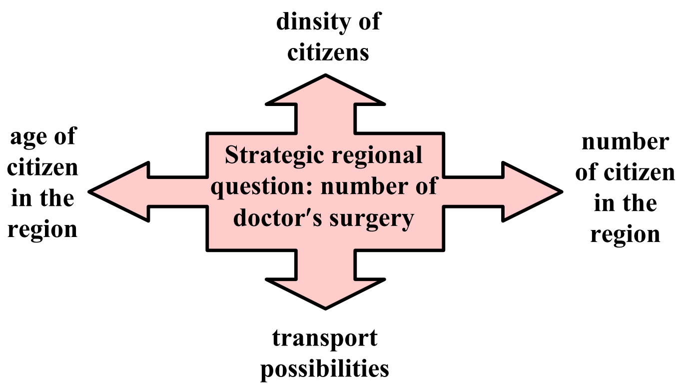

Fig. 4: Example of strategic question

We can show using of algorithm practically on simple example. Example above (see figure 5) shows three levels of solution. The first level (ad A) deals with analyzing of regional hospital (symbol H in the picture). We can find variously deployed municipalities around hospital round the hospital (black point around hospital). The municipalities are variously distant from hospital, municipalities have various number of citizens and various transport accessability to the hospital and. Every town has different population and different density domesticate. Every of these values we can use to the one's functional funds *f(x)* which we will assign to every municipalities. This is the second level (ad B) of analyzing of the problem. Then we can institute each value of a function to algorithm and reckon optimum distance to the different hospitals (ad C). The number C is becomingly elect criterion which we will use in algorithm. This criterion is reduced in every step and also the value of a function state *f(x)* is reduced. This new state is received then with definite probability. The curve of probability of new state undertaking *x`* is in the picture.

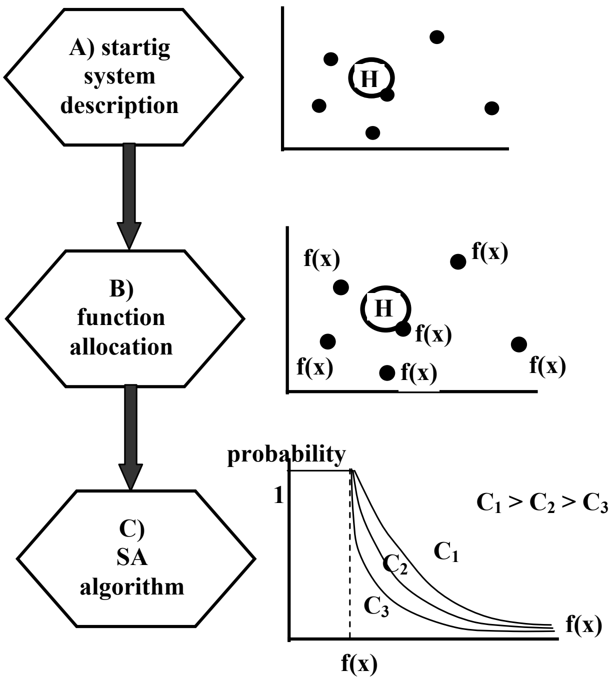

Fig. 5: Example of SA using

ad C)
1. procedure SA
2. set starting point $i = i_0$;
3. set starting criterion $C = C^0$ and cooling rate $0 < \alpha < 1$;
4. set N_T (number of trials per criterion);
5. while stopping condition is not satisfied do
6. for $k \leftarrow 1$ to N_T do
7. generate trial point i` from $S_i$ using q(i; i`);
8. accept i` with probability $A_C$ (i; i`)
9. end for
10. reduce criterion by $C \leftarrow \alpha \times C$;
11. end while
12. end procedure

4 Conclusion

Using of optimization methods is necessary for efficient managing of region. Regional sources of information contain huge number of data which hides large potential for answering of strategic regional inquiries. Management of regional institution often needs to find optimum with solving concrete problem if the optimum is contingent by various criteria. Funds of criteria are available in line time, structural rows and at others rows.

Method of SA offers possibility of very effective algorithm to solving combinatorial exercise and gained solutions are either identical or very near to optimum solution.

References:

[1] Bertsekas, D. P.: *Constrained Optimization and Lagrange Multiplier Methods*. Academic Press, 1982

[2] Luenberger, D. G.: *Linear and Nonlinear Programming*. Addison-Wesley Publishing Company, Reading, MA, 1984

[3] Nocedal, J., Wright, S. J.: *Numerical Optimization*. Springer – Verlag, New York. 1992

[4] Rardin, R. L.: *Optimization in Operations Research*. Upper Saddle River, New Jersey: Prentice Hall, 1998

[5] Humphries, M., Hawkins, M, W.: *Data warehousing – Architecture and implementation (Czech translation)* Computer Press Prague 2002

[6] Simonova, S., Capek, J. Fuzzy Approach in Enquiry to Regional Data Sources for Municipalities, *WSEAS TRANSACTIONS ON INFORMATION SCIENCE AND APPLICATIONS*, Vol.3, No.2, 2004, pp. 823-827.

[7] Ait-Aoudia, S., Mana I.: Numerical Solving of Geometric Constraints by bisection A Distributed Approach, WSEAS *TRANSACTIONS ON INFORMATION SCIENCE AND APPLICATIONS*, Vol. 1, No.5, 2004, pp. 1231-1236.