paper's category: genetic algorithm

Application of numerical optimization technique based on real-coded genetic algorithm to inverse problem in biochemical systems

Takanori Ueda
Graduate School of Bioresource and Bioenvironmental Sciences
Kyushu University
Fukuoka 812-8581, Japan
ueda@brs.kyushu-u.ac.jp

Nobuto Koga
Dept. of Biochem. Eng. & Sci.
Kyushu Institute of Technology
Fukuoka 820-8502, Japan
nob@brs.kyushu-u.ac.jp

Isao Ono
Faculty of Eng.
The University of Tokushima
Tokushima 770-8506, Japan
isao@is.tokushima-u.ac.jp

Masahiro Okamoto
Graduate School of Bioresource and Bioenvironmental Sciences
Kyushu University
Fukuoka 812-8581, Japan
okahon@brs.kyushu-u.ac.jp

Abstract

Real-coded Genetic Algorithms (RCGA) attract attention as numerical optimization methods for nonlinear systems. One of the crossover operators for RCGA called unimodal normal distribution crossover (UNDX) has shown good performance in optimization of various functions including multi-modal ones and benchmark functions with epistasis among parameters (Ono and Kobayashi, 1997). The UNDX generates new population lie on some ponds or along some valleys in order to focus the search on promising areas from a viewpoint of searching efficiency. Especially when the function has epistasis among parameters, namely valleys that are not parallel to coordinate axis, the UNDX can efficiently optimize it. Simple GA is one of the well-known generation alternation models, however, it has two problems. One is early convergence in the fast stage of search and the other is evolutionary stagnation in the last stage of it. A new generation alternation model called minimal generation gap (MGG) was proposed to overcome the above problems (Sato et al., 1997, Ono et al., 2000). The MGG has all advantages of convention models and the ability of avoiding the early convergence and suppressing the evolutionary stagnation.

Here, we applied the combination method (MGG+UNDX) to the optimization of real-valued parameters in the form of the S-system that is a type of power-law formalism and is suitable for description of organizationally complex systems such as gene expression networks (Maki et al., 2001) and metabolic pathways (nonlinear biochemical systems). The S-system is based on a particular type of ordinary differential equation in which such component processes are characterized by power-law functions as follows:

$$\frac{d}{dt}X_i = \alpha_i \prod_{j=1}^{n} X_j^{g_{ij}} - \beta_i \prod_{j=1}^{n} X_j^{h_{ij}} \qquad (1)$$

where n is the total number of state variables or reactants (X_i), i, j ($1 \le i,\ j \le n$) are suffixes of state variables. The terms g_{ij} and h_{ij} are interactive effectivity of X_j to X_i. The first term represents all influences that increase X_i, whereas the second term represents all influences that decrease X_i. In a reaction network context, the non-negative parameters α_i and β_i are called relative inflow and outflow of reactant X_j, and real-valued exponents g_{ij} and h_{ij} are referred to as the interrelated coefficients between reactants X_j and X_i. Since the S-system is a formalism of ordinary nonlinear differential equation, the system can easily be solved numerically by using a numerical calculation program to be customized specifically for this structures. However, when an adequate time-course of relevant state variable is given, a set of parameter values α_i, β_i, g_{ij} and h_{ij}, in many cases, will not be uniquely determined, because it is highly possible that the other sets of parameter values will also show a similar time-course. Therefore, even if one set of parameter values that matches the observed time-courses is obtained, this set is still one of the best candidates that explain the observed time-courses. Our strategy is to explore and exploit these candidates within the immense huge searching space of parameter values. In the results, MGG+UNDX showed superiority in searching eficiency to the simple GA as the precision of the optimization becomes higher.

Acknowledgement

This work was partially supported by the Grants-in-Aid for Scientific Research on Priority Areas (C), "Genome Information Sciences" (No.12208008) from the Ministry of Education, Culture, Sports, Science and Technology in Japan (MO).