Method for determining search states of Markov Chain practically and its application to predict EC convergence and proof it

Pei, Yan
Graduate School of Design, Kyushu University

Takagi, Hideyuki
Faculty of Design, Kyushu University

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マルコフ連鎖の探索状態決定方法とその進化計算収束予測と証明への応用

裴 岩[†], 高木英行[††],

九州大学大学院芸術工学府[†], 九州大学大学院芸術工学研究院[††],

1 Introduction and Related Works

Theoretical and applied studies are two aspects of evolutionary computation (EC) research in EC community. Most of the researches focus on the applied study, here the objective is to apply a variety of EC algorithms and techniques to real world optimization applications. A few of the researches are related to the theoretical and fundamental works of EC, the objective here is to establish formal approaches to prove the effectiveness and practicability of EC algorithms and techniques.

If a formal techniques can be considered as a search algorithm, it should confirm the following properties and characteristics [1)].

1. Complete: if it guarantees reaching a terminal state/solution if there is one.
2. Optimal: if the solution is found with the optimal value of its objective function.
3. Search Optimal: if the solution is found with the minimal amount of resources used (e.g., the time and space complexity).
4. Totally Optimal: if the solution is found both with the optimal value of its objective function and with the minimal amount of resources used.

EC convergence research (including complete and optimal properties mentioned above) is one of the EC theoretical researches. There are main two EC convergence analysis methods that have been proposed in EC community, i.e., fixed point theory by Michael D. Vose [5)] and Markov analysis by David E. Goldberg [2, 4)] .

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[†] Yan PEI(peiyan@kyudai.jp)
[††] Hideyuki TAKAGI(takagi@design.kyushu-u.ac.jp)
Graduate School of Design, Kyushu University (†)
Faculty of Design, Kyushu University (††)

The fixed point theory of EC convergence study is only using the simple genetic algorithm (GA) as a research model. The philosophy of this approach is to apply two matrix operators (selection operator and recombination operator) to describe simple GA search process, and it studies two fixed points of the two matrix operators to analyze on GA's convergence [5)] .

The EC population state depends on its last population information, and does not relate to the state and information before the last population, therefore Markov chain is a natural method to describe the EC's convergence . However, the drawback of Markov analysis works is that there is not a general and explicit definition and explanation for system state definition and transition probability matrix. Any stochastic sampling algorithm can use Markov analysis method to obtain the convergence or no convergence result.

In this paper, we proposal to use fitness transition state to study on the convergence characteristic of EC algorithm by Markov chain rather than using the states of parameter space (population state). A method of determining search state by fitness in Markov chain is defined. One and n step state transition matrices are established to study on the convergence of EC algorithms. From an empirical study, the proposed method can be used as a analysis tool to predict and proof the convergence of EC algorithm.

Following this introduction and overview of the some theoretical works of EC, a review of fundamental knowledge about Markov Chain is presented in section 2. In this paper, we define an EC algorithm search state by fitness space and establish one-step and n-step transition probability matrix based on this definition to analyze the EC algorithm convergence in section 3. We also discuss EC algorithm's ergodicity by finite Markov chains, and an empirical study of our evaluation results is involved in section 4. Finally, we conclude the whole in section 5.

2 Markov Chain Fundamental

In general, Markov chain is a tool to describe the stochastic process that the state of the future only depends on the current state and absolutely does not relate to the state in the current before. Supposed that there is a stochastic process $X(t), t \in T$ and its state space is I, if Eq.(1) condition holds true, we can call that this stochastic process is with the property of Markov, or it is a Markov process.

$$\begin{aligned} P\{X(t_n)|X(t_1) = x_1, X(t_2) = x_2, ..., X(t_{n-1}) = x_{n-1}\} \\ = P\{X(t_n)|X(t_{n-1}) = x_{n-1}\} \end{aligned} \tag{1}$$

If time and state of the stochastic process are from the discrete space, it is called as a Markov chain.

2.1 Transition Probability and One-Step Transition Probability Matrix

The transition probability of Markov chain describes the probability when a stochastic process transfer from state = a_i and time = m to state = a_j and time = $m+n$, as shown in Eq. (2) .

$$P_{ij}(m, m+n) = P\{X_{m+n} = a_j | X_m = a_i\} \tag{2}$$

It is called as a one-step transition probability matrix that is a matrix made by the transition probability (Eq. 3).

$$P(1) = \begin{bmatrix} p_{11} & p_{12} & \cdots & p_{1j} \\ p_{21} & p_{22} & \cdots & p_{2j} \\ \cdots & \cdots & \cdots & \cdots \\ p_{i1} & p_{i2} & \cdots & p_{ij} \end{bmatrix} \tag{3}$$

2.2 Chapman-Kolmogorov Equation and n-Step Transition Probability Matrix

Chapman-Kolmogorov equation is the basic rule when making a n-step transition probability matrix (Eq. (4)).

$$P_{ij}(u+v) = \sum_{k=1}^{\infty} P_{ik}(u) P_{kj}(v) \tag{4}$$

It indicates that the probability of state in the time = $s+u+v$ ($X(s+u+v)$) is the result of the AND operation first from $X(s) = a_i$ to $X(s+u) = a_k$, and then to $X(s+u+v) = a_j$ (Fig. (1)). We can use the Chapman-Kolmogorov equation to obtain the n-step transition probability matrix from a one-step transition probability matrix.

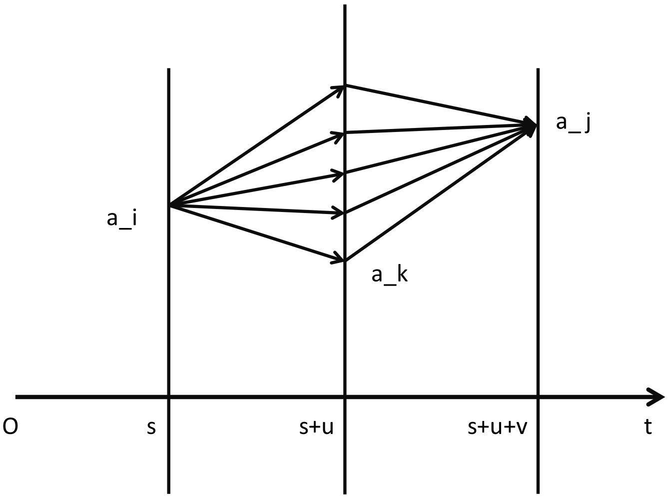

Fig. 1 Chapman-Kolmogorov Equation and n-Step Transition Probability Matrix.

3 Our Proposal: A New Definition of Markov Chain Search State

3.1 A Brief Overview Conventional Analysis and Our Proposal

There are two kinds of spaces in EC algorithms, the one is a parameter space and the other is a fitness space, surely, if it is a multi-objective EC algorithm, the fitness space is more than one. The conventional analysis method of EC convergence establishes a Markov chain with the parameter space and study on the states of fitness space (a hidden chain) by hidden Marfov chain technique. It predicts the state of hidden chain in fitness space from the explicit states of Marfov chain in parameter space. This presents a the study philosophy of conventional analysis method.

Beside the two chains in conventional analysis method, we propose a third chain that simplifies the states of fitness space, and study search condition from the sequences such as: fitness transition space, fitness space and parameter space. There are two hidden Markov chains in this analysis process. If one hidden Marfov chain can be shortened for HM, the proposed method is HM^2. Fig. 2 sketches the main philosophies of conventional analysis method and our proposal.

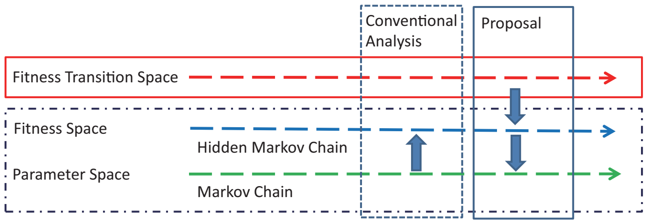

Fig. 2 Conventional analysis method of EC convergence and our proposal.

3.2 Definition of Search State

The first step of our analysis method is to define a search state of EC algorithm by fitness space state. Different from defining real system outputs as the system state, we propose to use the system transfer states as a basic states to establish a transition probability matrix. For non-divergence algorithms, there must be two states in the running process of algorithm . Taking a minimum optimal problem as an instance, there are two states: fitness improvement (except convergence) and fitness stagnation (besides convergence) (Eq. (5)). We use these two basic states to establish a transition probability matrix.

$$SearchState = \{Improvement, Stagnation\} \tag{5}$$

3.3 Transition Probability Matrix

Based on the definition of EC search state, we should count the state transition times of (1) improvement to improvement; (2) improvement to stagnation; (3) stagnation to improvement and (4) stagnation to stagnation, and we establish the one-step transition probability matrix as in Eq. (6).

$$P(1) = \left[\begin{array}{c|cc} & Improvement & Stagnation \\ \hline Improvement & \frac{(1)}{(1)+(3)} & \frac{(2)}{(2)+(4)} \\ Stagnation & \frac{(3)}{(3)+(1)} & \frac{(4)}{(4)+(2)} \end{array}\right] \tag{6}$$

According to the Chapman-Kolmogorov equation (Eq. (4)), the n-step transition probability matrix is given by Eq. (7). We use n-step transition probability matrix to study EC Ergodicity and give its convergence condition.

$$P(n) = P(1)^n \tag{7}$$

3.4 Ergodicity

As the same as the other guided random algorithms, the EC iteration process can be described as a finite Markov chain. For a finite Markov chain, there is a theorem that shows its ergodicity.

- **Theorem1**: For finite Markov chains $\{X_n, n \geq 1\}$ with the state space is $I = \{a_1, a_2, \ldots, a_N\}$, if P is its one-step transition probability matrix, $\forall\ m \in R^+$, and $a_i, a_j \in I$, $\exists\ P_{ij}(m) > 0$, this finite Markov chains is with ergodicity. And, the distribution of the limit is the unique solution of equation system Eq. (8).

$$\begin{aligned} &\pi_j = \sum_{i=1}^{N} \pi_i p_{ij} \\ &\pi_j > 0 \\ &\sum_{j=1}^{N} \pi_i = 1 \end{aligned} \tag{8}$$

4 An Empirical Study

To further investigate our proposed EC convergence analysis approach performance, we select the evaluation data from our recent work as a sample, which uses the CE-4 method optimizes F1 function [3)]. We calculate the related data to establish its one-step and n-step transition probability matrix by Eq. (6) and Eq. (7) to study its ergodicity and convergence performance.

Eq. (9) shows one-step transition probability matrix of the F1 function optimized by the CE-4 method. By the **Theorem1**, all the elements of this matrix are more than zero, it shows the CE-4 method has the ergodic property, i.e., its limited probability distribution exists. We calculate the n-step transition probability matrix ($n = 10^5$) to obtain the approximated probability value in Eq. (10), where it shows that whatever the initial state of CE-4 method, it can obtain the stagnation state to the stagnation state with the probability equal 0.9995.

It indicates that, for a landscape with the characteristic of F1 function (a big valley structure), CE-4 can converge with probability of 0.9995 in general. We can use this conclusion to predict and proof that when applying the CE-4 method to a landscape as the same as F1, it can converge with probability of 0.9995.

$$P(1)=\left[\begin{array}{c|cc} & \mathit{Improvement} & \mathit{Stagnation} \\ \hline \mathit{Improvement} & 0.944202899 & 2.54075E-05 \\ \mathit{Stagnation} & 0.055797101 & 0.999974592 \end{array}\right] \tag{9}$$

$$P(10^5)=\left[\begin{array}{c|cc} & \mathit{Improvement} & \mathit{Stagnation} \\ \hline \mathit{Improvement} & 0.0005 & 0.0005 \\ \mathit{Stagnation} & 0.9995 & 0.9995 \end{array}\right] \tag{10}$$

5 Conclusion and Future Works

We propose a new definition of EC search state to establish a new analysis method of EC convergence based on Markov chain, and use an empirical experimental data to evaluate the proposal. The future work will involve the topics on the effectiveness of the proposal from more real world application, the EC algorithm convergence prediction accuracy in the problems with a variety of landscapes. We will conduct these works in the future.

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