A Unified Markov Chain Approach to Analysing Randomised Search Heuristics

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Abstract

The convergence, convergence rate and expected hitting time play fundamental roles in the analysis of randomised search heuristics. This paper presents a unified Markov chain approach to studying them. Using the approach, the sufficient and necessary conditions of convergence in distribution are established. Then the average convergence rate is introduced to randomised search heuristics and its lower and upper bounds are derived. Finally, novel average drift analysis and backward drift analysis are proposed for bounding the expected hitting time. A computational study is also conducted to investigate the convergence, convergence rate and expected hitting time. The theoretical study belongs to a prior and general study while the computational study belongs to a posterior and case study.

1 Introduction

Randomised search heuristics, such as evolutionary algorithms, have been widely applied to optimization problems. Randomised search heuristics belong to iterative methods. As iterative methods, the following three questions are fundamental in both theory and practice.

1. (Convergence) whether is a randomised search heuristic able to find an optimal solution eventually?
2. (Convergence rate) how fast does a randomised search heuristic converge to the optimal set per iteration?
3. (Hitting time) how many iterations are needed for obtaining an optimal solution?

Most randomised search heuristics satisfy the Markov property, that is, a population sequence (where a population consists of one or more solutions) is generated subject to some probability distribution; and the state of current population decides the state of next population in a probabilistic way. Hence Markov chain theory provides a theoretical framework for analysing randomised search heuristics [31, 18].

Based on absorbing Markov chain theory [22, 13], a unified approach is used for studying the convergence, convergence rate and expected hitting time of randomised search heuristics in this paper. The idea is described as follows: the population sequence generated by a randomised search heuristic is modelled by an absorbing Markov chain. Consider the probability distribution of a population in the non-optimal solution set and represent it by a vector. Then the randomised search is equivalent to a matrix iteration. The vector 1-norm is chosen to measure the distance between a population and the optimal solution set. This new feature makes our current analysis different from previous work [30, 34, 15]. Using matrix iteration analysis [35, 24], all theoretical results can be established in a unified manner.

The purpose of this paper is to seek new theoretical tools for analysing randomised search heuristics. Indeed we have developed three new tools in the paper, which are novel average drift analysis and novel backward drift analysis for bounding the expected hitting time; and the average convergence rate of randomised search heuristics. These new tools are seldom studied before.

This paper is organised as follows: literature review is given in Section 2. The Markov chain model appears in Section 3. Convergence is analysed in Section 4. The average convergence rate of EAs is discussed in Section 5. The expected hitting time is analysed in Section 6. Final conclusions are described in Section 7.

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2 Literature Review

In this section we review the work related to Markov chain analysis for randomised search heuristics, and also show the difference between our work and previous ones.

Markov chains have been applied into analysing randomised search heuristics more than two decades \cite{12,10}. \cite{31} gave a survey of Markov chain analysis of evolutionary algorithms up to 1998. \cite{29} reviewed some achievements after that year.

Markov chain theory provides a theoretical framework to model randomised search heuristics. For example, \cite{27,4,5} modelled genetic algorithms by Markov chains. \cite{2} presented Markov chain models of parallel genetic algorithms. In general, randomised search heuristics for discrete optimisation may be modelled by Markov chains, and randomised search heuristics for continuous optimisation by Markov processes.

Markov chain theory is widely applied to the limit behaviour of randomised search heuristics and their convergence. For example, \cite{11,30,19} proposed different convergent conditions of genetic algorithms. \cite{32} analysed convergence properties of some multi-objective evolutionary algorithms. \cite{3} compared various selection algorithms using Markov chains.

The convergence rate of randomised search heuristics is a less studied topic. \cite{34} analysed a simple GA by evaluating the eigenvalues of the transition matrix of the Markov chain and computed its convergence rate. \cite{15} gave the convergence rates of general genetic algorithms by using the minorization condition. \cite{9} studied the convergence rates of gene expression programming by means of Markov chain and spectrum analysis.

The expected hitting time study has received more attentions recently. \cite{16,8} made two initial discussions on evolutionary algorithms. According to absorbing Markov chain theory, the expected hitting time can be calculated based on the fundamental matrix. Using this approach, \cite{17} compared the expected hitting time of (1 + 1) and (N + N) evolutionary algorithms. \cite{18} gave a framework for analysing the expected hitting time of evolutionary algorithms. \cite{37} compared the runtime of three simple heuristic algorithms.

However, the fundamental matrix approach can only be suitable for simple algorithms and problems. Thus \cite{14,16} introduced drift analysis to the expected hitting time study. Currently drift analysis becomes a popular theoretical tool. Different variants have been developed, such as simplified drift analysis \cite{28}, multiplicative drift analysis \cite{7}, adaptive drift analysis \cite{6}, and variable drift \cite{25,21}. Drift analysis have been applied to both (1+1) EAs \cite{36} and population-based EAs \cite{23}. Drift theorems can be established using either Markov chain theory or super-martingale theory \cite{16,26}.

So far the convergence, convergence rate and expected hitting time are studied separately. Different from existing work, we present a unified approach to bringing these three issues together.

3 Absorbing Markov Chain Model

3.1 Theoretical Study

In this subsection, we describe absorbing Markov chain models of randomised search heuristics.

Consider a maximisation problem on a finite state space, that is

\[ \max f(x), \quad x \in D, \]  

where \( x \) is a variable and \( D \) is its definition domain, a finite set. \( f(x) \) is called a fitness function.

A randomised search heuristic can be viewed as a randomised iteration process: initially construct a population of solutions \( \Phi_0 \); based on \( \Phi_0 \), then probabilistically generate a new population of solutions \( \Phi_1 \); based on \( \Phi_1 \), then probabilistically generate a new population of solutions \( \Phi_2 \), and so on. This procedure is repeated until a stopping criterion is satisfied. Then a sequence of populations is produced \( \Phi_0 \rightarrow \Phi_1 \rightarrow \Phi_2 \rightarrow \cdots \).

In order to guarantee that the best solution is always kept during the iteration, an extra archive is added for recording the best found solution. The archive itself is not involved in generating new solutions. This strategy is called elitist. A randomised search heuristic with an archive is described in Algorithm 1.

A population consists of one or more solutions while a solution is called an individual. The procedure of generating new a population may include several steps, such as mutation, crossover and selection in a genetic
In this subsection, we show how randomised heuristics can be easily modelled by Markov chains. For the sake of illustration, we consider a simple maximisation problem

\[ \text{max } f(x), \quad x \in \{0, 1, \cdots, 100\} \]  

Two randomised search heuristics are applied to the above problem. The first algorithm adopts random walk with elitist selection, denoted by RSH-I (see Algorithm 2).

**Algorithm 1** randomised search heuristic with an archive

1: set counter \( t \) to 0;
2: initialize a population of solutions \( \Phi_0 \);
3: archive \( \Lambda_0 \) keeps the best solution in \( \Phi_0 \);
4: for \( t = 0, 1, 2, \cdots \) do
5: \hspace{1em} a new population of solutions \( \Phi_{t+1} \) is generated from \( \Phi_t \);
6: \hspace{1em} update the archive \( \Lambda_{t+1} \) if the best solution in \( \Phi_{t+1} \) is better than \( \Lambda_t \);
7: \hspace{1em} counter \( t \) is increased by 1;
8: end for

algorithm. For convenience of analysis, we only consider non-dynamical algorithms whose search operators are not changed during the iteration. The algorithm runs for ever. This assumption is taken for convenience of analysis of the hitting time. The fitness of a population at the \( t \)-th iteration is defined by the archive at the \( t \)-th iteration, denoted by \( f_t \).

The sequence \( \{ \Phi_t; t = 0, 1, \cdots \} \) can be formulated by a Markov chain. Let \( X \) and \( Y \) be two populations. The transition from \( X \) to \( Y \) happens with a probability \( P(X, Y) \), that is,

\[ P(X, Y) := P(\Phi_{t+1} = Y | \Phi_t = X), \quad X, Y \in S, \]  

where \( S \) denotes the set of all populations. Both \( \Phi_t \) and \( X \) represent a population, but \( \Phi_t \) is a random variable for representing the population at the \( t \)-th iteration; \( X \) its value, or called a state in the population space.

For the sake of argument, we introduce an auxiliary Markov chain \( \{ \Phi'_t; t = 0, 1, \cdots \} \) as follow. Let \( \Phi'_t = \Phi_t \) before the optimal solution is found for the first time. Once an optimal solution is found at the \( t \)-th iteration, then assign \( \Phi'_t = \Phi_t \) for any iteration \( s \) after \( t \). This implies the optimal set is always absorbing in the new chain \( \{ \Phi'_t; t = 0, 1, \cdots \} \). We don’t care about the behaviour of randomised search heuristics after the first time to hit an optimal solution. To simplify notation, we still denote the new chain by \( \{ \Phi_t; t = 0, 1, \cdots \} \). As a result, the population sequence \( \{ \Phi_t; t = 0, 1, \cdots \} \) is modelled by a homogeneous Markov chain where the optimal solution set is always absorbing.

### 3.2 Case Studies

In this subsection, we show how randomised heuristics can be easily modelled by Markov chains. For the sake of illustration, we consider a simple maximisation problem

[\text{max } f(x), \quad x \in \{0, 1, \cdots, 100\}]  

Two randomised search heuristics are applied to the above problem. The first algorithm adopts random walk with elitist selection, denoted by RSH-I (see Algorithm 2).

**Algorithm 2** RSH-I

**Random Walk**: provided that \( \Phi_t = x \), then it walks to \( x - 1 \) (if \( x - 1 \) is not less than 0) with probability 0.01, or walks to \( x + 1 \) (if \( x + 1 \) is not more than 100) with probability 0.01. Denote the new position by \( \Phi_{t+1}/2 \).

**Elitist Selection**: if \( f(\Phi_{t+1}/2) > f(\Phi_t) \), then let \( \Phi_{t+1} \leftarrow \Phi_{t+1}/2 \); otherwise \( \Phi_{t+1} \leftarrow \Phi_t \).

The sequence \( \{ \Phi_t; t = 0, 1, \cdots \} \) is a Markov chain and its transition probabilities are given as follows: for any \( x, y \in \{0, 1, \cdots, 100\} \) which are not in the optimal solution set,

\[ P(x, y) = \begin{cases} 0.01, & \text{if } y = x - 1 \text{ and } f(y) > f(x); \\ 0.01, & \text{if } y = x + 1 \text{ and } f(y) > f(x); \\ p, & \text{if } y = x; \\ 0, & \text{otherwise.} \end{cases} \]

where \( p = 1 - P(x, x - 1) - P(x, x + 1) \).
Thus the convergence of a randomised search heuristic is rewritten in the norm form:

\[ \lim_{t \to +\infty} \| \Phi_t \|_1 = 0. \]

The second algorithm adopts random walk with non-elitist selection, denoted by RSH-II (see Algorithm 3). Different from RSI-I, RSH-II allows a worse child to be accepted.

\[ P(x, y) = \begin{cases} 
0.01, & \text{if } y = x - 1 \text{ and } f(y) > f(x); \\
0.005, & \text{if } y = x - 1 \text{ and } f(y) \leq f(x); \\
0.01, & \text{if } y = x + 1 \text{ and } f(y) > f(x); \\
0.005, & \text{if } y = x + 1 \text{ and } f(y) \leq f(x); \\
p, & \text{if } y = x; \\
0, & \text{otherwise}; 
\end{cases} \]

where \( p = 1 - P(x, x - 1) - P(x, x + 1) \).

4 Convergence in Distribution

4.1 Theory Study: Convergence Condition

In this subsection we define the convergence in distribution of randomised search heuristics and establish the sufficient and necessary conditions of convergence in distribution.

Let \( S_{\text{opt}} \) denote the set of all populations which includes at least one optimal solution, and \( S_{\text{non}} \) the set of all populations which doesn’t include any optimal solution.

**Definition 1.** A randomised search heuristic is called convergence in distribution if starting from any non-optimal population, the probability of \( \Phi_t \) in the optimal set goes towards 1 as \( t \) to the infinitely large. That is

\[ \lim_{t \to +\infty} P(\Phi_t \in S_{\text{opt}}) = 1. \]

We consider the probability distribution of \( \Phi_t \) in the non-optimal set. Let \( q_t(X) \) denote the probability of \( \Phi_t \) at a non-optimal state \( X \),

\[ q_t(X) := P(\Phi_t = X). \]

Let \((X_1, X_2, \cdots)\) represent all populations in the non-optimal set. Then the vector\(^2\) \( q_t \)

\[ q_t := (q_t(X_1), q_t(X_2), \cdots)^T \]

denote the probability distribution of \( \Phi_t \) over all non-optimal populations.

Notice that the vector 1-norm\(^1\) \( \| q_t \|_1 = P(\Phi_t \in S_{\text{non}}) \).

Thus the convergence of a randomised search heuristic is rewritten in the norm form:

\[ \lim_{t \to +\infty} \| q_t \|_1 = 0. \]

\(^1\)Notation \( \mathbf{v} \) represents a column vector and \( \mathbf{v}^T \) the row column with the transpose operation.

\(^2\)Given an \( n \times n \) matrix \( \mathbf{A} = [a_{i,j}] \), its 1-norm is \( \| \mathbf{A} \|_1 = \max_{1 \leq j \leq n} \sum_{i=1}^n | a_{ij} | \). Given a vector \( \mathbf{v} \), its 1-norm is \( \sum_{i=1}^n | v_i | \).
The 1-norm \( \| q_t \|_1 \) plays the role of the distance between the population \( \Phi_t \) and the optimal set. This can be viewed as a special case of the analysis in [13], where a general vector norm has been used as the distance.

In the following we draw the convergence condition of randomised search heuristics based on the absorbing Markov chain theory.

Let \( P \) denote the transition matrix of the Markov chain associated with a randomised search heuristic, whose entries are \( P(X, Y) \), where \( X, Y \in S \). Since a state in the optimal set is always absorbing, so the transition matrix \( P \) can be written in the canonical form below,

\[
P = \begin{pmatrix}
  I & O \\
  R & Q
\end{pmatrix},
\]

where \( I \) is a unit matrix and \( O \) a zero matrix. \( Q \) is a matrix to denote probability transitions among non-optimal populations. \( R \) is a matrix to represent probability transitions from non-optimal populations to the optimal set.

According to absorbing Markov chain theory [13, Chapter 11],

\[
P(\Phi_{t+1} = Y) = \sum_{X \in S_{\text{non}}} P(\Phi_t = X)P(X, Y),
\]

then the iteration \( \Phi_t \rightarrow \Phi_{t+1} \) is represented in an equivalent matrix iteration,

\[
q_{t+1}^T = q_t^T Q = q_0^T Q^t.
\]

From the sufficient and necessary condition of convergence of iterative methods ([35, Theorem 1.10]), it is straightforward to obtain the convergence condition for randomised search heuristics:

**Lemma 1.** A randomised search heuristic is convergent if and only if the spectral radius \( \rho(Q) < 1 \).

The above sufficient and necessary condition is less useful in practice since it is too difficult to calculate the spectral radius of the transition matrix. Therefore we turn to find an equivalent condition which is much easier to verify. The following lemma gives such a condition.

**Lemma 2.** A randomised search heuristic is convergent if and only if starting from any non-optimal population, it is possible to visit the optimal set after finite iterations. That is, there exists an integer \( k > 0 \) and for any non-optimal state \( X \) and \( t \geq 0 \),

\[
P(\Phi_{t+k} \in S_{\text{opt}} | \Phi_t = X) > 0.
\]

**Proof.** Since the chain \( \{ \Phi_t : t = 0, 1, \cdots \} \) is homogeneous, thus it is enough to prove the case of \( t = 0 \).

(i) The proof that the condition is sufficient.

Assume \( (\star) \) holds. From

\[
P(\Phi_k \in S_{\text{non}} | \Phi_0 = X) + P(\Phi_k \in S_{\text{opt}} | \Phi_0 = X) = 1,
\]

then it gives \( \| q_k \|_1 < 1 \) for any \( \| q_0 \|_1 \) such that \( \| q_0 \|_1 = 1 \).

Then from the matrix iteration \( q_k = (Q^T)^k q_0 \), and the matrix 1-norm definition

\[
\| (Q^T)^k q_0 \|_1 = \max_{\| q_0 \|_1 = 1} \| (Q^T)^k q_0 \|_1,
\]

it follows

\[
\| (Q^T)^k \|_1 < 1.
\]

Since the spectral radius of a matrix is never bigger than its consistent norm [24, Example 7.1.4], the above inequality yields

\[
\rho((Q^T)^k) \leq \| (Q^T)^k \|_1 < 1,
\]

The spectral radius of a square matrix \( A \), denoted by \( \rho(A) \), is the supremum among the absolute values of all eigenvalues of \( A \).
so that $\rho(Q) = \rho(Q^T) < 1$. According to Lemma 1, this implies that the algorithm is convergent.

(ii) The proof that the condition is necessary.

Suppose the algorithm is convergent, then according to Lemma 1, $\rho(Q) = \rho(Q^T) < 1$. From Gelfand’s spectral radius formula\(^4\) there exists an integer $k > 0$ such that

\[
\| (Q^T)^k \|_1^{1/k} < 1.
\]

and then $\| (Q^T)^k \|_1 < 1$.

From $q_k = (Q^T)^k q_0$, it gives $\| q_k \|_1 < 1$.

From

\[
P(\Phi_k \in S_{\text{non}} \mid \Phi_0 = X) + P(\Phi_k \in S_{\text{opt}} \mid \Phi_0 = X) = 1,
\]

and

\[
\| q_k \|_1 = P(\Phi_k \in S_{\text{non}} \mid \Phi_0 = X),
\]

It follows then that

\[
P(\Phi_k \in S_{\text{opt}} \mid \Phi_0 = X) > 0,
\]

and this proves (6).

From the above lemma, we can easily draw the following sufficient and necessary condition, which is much easier to verify in practice.

**Theorem 1.** A randomised search heuristic is convergent if and only if starting from any non-optimal state, it is possible to reach a better state after finite iterations. That is, there exists an integer $k > 0$ and for any non-optimal state $X$ and $t \geq 0$,

\[
P(f_{t+k} > f_t \mid \Phi_t = X) > 0.
\]

### 4.2 Case Study

In this subsection, we show how the convergence conditions are applied to determine the convergence of a randomised search heuristic.

**Example 1.** Consider RSH-I and RSH-II for solving the following maximisation problem,

\[
\max f(x), \quad x \in \{0, 1, \cdots, 100\}.
\]

RSH-I does not converge if there exists a state $x$ such that $f(x) > f(x - 1)$ and $f(x) > f(x + 1)$. This means $f(x)$ is a multi-modal function. At the local optimum $x$, the algorithm cannot make any move.

RSH-II always converges. It is easy to verify that from any state $X$, the algorithm can make an improvement at most 100 iterations with a positive probability, thus according to Theorem 1 the algorithm is not convergent.

**Example 2.** Consider RSH-I for solving the following maximisation problem

\[
\max x^2, \quad x \in \{0, 1, \cdots, 100\}.
\]

It is a unimodal function with the optimum at 100.

The corresponding transition matrix $Q$ is

\[
Q = \begin{pmatrix}
0.99 & 0 & \cdots & 0 & 0 \\
0.01 & 0.99 & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & 0.99 & 0 \\
0 & 0 & \cdots & 0.01 & 0.99 \\
\end{pmatrix}.
\]

---

\(^4\)Gelfand’s spectral radius formula says that for any induced matrix norm: $\lim_{t \to +\infty} \| A^k \|^{1/k} = \rho(A)$ [24, Example 7.10.1].
We can prove the convergence of RSH-I using Lemma 1. Since \( \rho(Q) = 0.99 < 1 \), so RSH-I for maximising \( f_1(x) \) is convergent.

We also can prove the convergence of RSH-I using Theorem 1 without calculating the spectral radius. It is easy to see that the probability of obtaining a better child is 0.01, thus according to Theorem 1, the algorithm is convergent.

Comparing with the two approaches, we see that Theorem 1 provides a faster approach to determine the convergence.

4.3 Computational Study

In this subsection, we propose a computational approach to illustrating the convergence in distribution of randomised search heuristics.

In the computation study, we run an algorithm for \( k \) times. Let \( n(\Phi_t \in S_{opt}) \) denote the number of \( \Phi_t \) (where \( t = 0, 1, \cdots \)) appearing in the optimal set for these \( k \) runs.

According to the law of large numbers, the probability \( P(\Phi_t \in S_{opt}) \) will be approximated by the relative frequency as follows:

\[
\frac{n(\Phi_t \in S_{opt})}{k}, \quad \text{when} \ k \to +\infty.
\]

The above frequency is used as the probability \( P(\Phi_t \in S_{opt}) \) in the computational study.

Example 3. Consider RSH-II for solving the following problem

\[
\max (x - 49)^2, \quad x \in \{0, 1, \cdots, 100\}. \tag{12}
\]

It is a two-modal function, with one local optimum at 0 and one global optimum at 100.

We apply RSH-I to the problem. Run the algorithm for 100,000 times. The initial population is \( \Phi_0 = 20 \). Figure 1 shows the probability of \( \Phi_t \) in the optimal set is 0 when \( t \leq 100,000 \). In other words, no convergence happens yet in 100,000 iterations.

![Figure 1: The probability \( P(\Phi_t \in S_{opt}) \) when RSH-I maximises \((x - 49)^2\).

Our approach is different from that of visualising the fitness value over \( t \). The latter approach may be the most popular used for illustrating the convergence of randomised search heuristics (for example, see Figures 1 to 3 in [1]). Figure 2 shows the fitness value \( f_t \) ‘converges’ after about 5,000 iterations and thereafter no change.

In Figure 2, RSH-I seems convergent, but this is only a kind of premature convergence to the local optimum at 0, rather than the global optimum at 100. In fact, the solution becomes farther away from the global optimum using the Euclidean distance: initially the distance between the solution and the optimum is \( 100 - 20 = 80 \); then after 6000 iterations, the distance increases to \( 100 - 0 = 100 \).

The approach of using the convergence in distribution provides a more accurate description of convergence than that of visualising the fitness value does.
5 Convergence Rate

5.1 Theoretical Study: Average Convergence Rate

In this subsection, we define the average convergence rate of randomised search heuristics and then present lower and upper bounds on the average convergence rate. The convergence rate is how fast a randomised search heuristic converges to the optimal set per iteration. It is an important measure of the performance of randomised search heuristics, but less studied.

Since randomised search heuristics belong to iterative methods, we adopt the average convergence rate, commonly used in iterative methods [35, Definition 3.1].

Definition 2. Assume the probability of the initial population $\Phi_0$ in the non-optimal set is larger than 0. The average rate of convergence for $t$ iterations is given by the following logarithmic reduction:

$$-\frac{1}{t} \ln \frac{\|q_t\|_1}{\|q_0\|_1}.$$  \hfill (13)

Since $P(\Phi_t \in S_{\text{non}}) = \|q_t\|_1$, then the average convergence rate for $t$ iterations can be rewritten as

$$-\frac{1}{t} \ln \frac{P(\Phi_t \in S_{\text{non}})}{P(\Phi_0 \in S_{\text{non}})}.$$  \hfill (14)

In the above definition, we don’t consider the case of the initial population in the optimal set with probability 1. In this case the algorithm already converges and no need to discuss the convergence rate.

Notice that

$$\frac{\|q_t\|_1}{\|q_0\|_1} = \frac{\|q_t\|_1}{\|q_{t-1}\|_1} \frac{\|q_{t-1}\|_1}{\|q_{t-2}\|_1} \cdots \frac{\|q_0\|_1}{\|q_0\|_1},$$

and the average convergence rate is equal to the logarithmic mean

$$-\frac{1}{t} \ln \frac{\|q_t\|_1}{\|q_0\|_1} = -\frac{1}{t} \left( \ln \frac{P(\Phi_t \in S_{\text{non}})}{P(\Phi_{t-1} \in S_{\text{non}})} + \cdots + \ln \frac{P(\Phi_1 \in S_{\text{non}})}{P(\Phi_0 \in S_{\text{non}})} \right).$$

The last formula shows that the average convergence rate is the average reduction factor of the probability of $\Phi_t$ in the non-optimal set per iteration in terms of the logarithmic mean.

In the following we estimate the lower bound and upper bound of the average convergence rate. The following theorem gives a lower bound on the average convergence rate.
Theorem 2. If a randomised search heuristic is convergent, then the averaged convergence rate is lower-bounded by

\[- \frac{1}{t} \ln \frac{\|q_t\|_1}{\|q_0\|_1} \geq - \frac{1}{t} \ln \| (Q^T)^t \|_1, \]  
\[- \lim_{t \to +\infty} \frac{1}{t} \ln \frac{\|q_t\|_1}{\|q_0\|_1} \geq - \ln \rho(Q). \tag{16} \]

Proof. From the matrix iteration \(q_t = (Q^T)^t q_0\), we get

\[\frac{1}{t} \ln \frac{\|q_t\|_1}{\|q_0\|_1} = \frac{1}{t} \ln \frac{\| (Q^T)^t q_0 \|_1}{\|q_0\|_1} \leq \frac{1}{t} \ln \| (Q^T)^t \|_1.\]

Then the first conclusion is proven.

Let \(t \to +\infty\) and apply Gelfand’s spectral radius formula, then

\[\lim_{t \to +\infty} \frac{1}{t} \ln \| (Q^T)^t \|_1 = \ln \rho(Q^T) = \ln \rho(Q).\]

Thus we prove that

\[- \frac{1}{t} \ln \frac{\|q_t\|_1}{\|q_0\|_1} \geq - \ln \rho(Q).\]

We prove the second conclusion.

Theorem 3. If a randomised search heuristic is convergent, then the average convergence rate is upper-bounded by

\[- \frac{1}{t} \ln \frac{\|q_t\|_1}{\|q_0\|_1} \leq - \frac{1}{t} \ln \left( \| (Q^T)^t \|_1 \right)^{-1}, \]  
\[- \lim_{t \to +\infty} \frac{1}{t} \ln \frac{\|q_t\|_1}{\|q_0\|_1} \leq \ln \rho(Q^{-1}) \tag{18} \]

Proof. From \(q_t = (Q^T)^t q_0\), we get

\[q_0 = ((Q^T)^{-1})^t q_t,\]

Hence

\[\|q_0\|_1 \leq \|((Q^T)^{-1})^t\|_1 \|q_t\|_1,\]
\[\|q_0\|_1 \|q_t\|_1 \leq \|((Q^T)^{-1})^t\|_1,\]

then

\[- \frac{1}{t} \ln \frac{\|q_t\|_1}{\|q_0\|_1} \leq - \frac{1}{t} \ln \left( \| ((Q^T)^{-1})^t \|_1 \right)^{-1}.\]

Then the first conclusion is proven.

According to Gelfand’s spectral radius formula and the fact \(\rho((Q^T)^{-1}) = \rho(Q^{-1})\), we get

\[\lim_{t \to +\infty} \left( \| ((Q^T)^{-1})^t \|_1 \right)^{1/t} = \rho((Q^T)^{-1}) = \rho(Q^{-1}).\]

Then

\[- \lim_{t \to +\infty} \frac{1}{t} \ln \frac{\|q_t\|_1}{\|q_0\|_1} \leq \ln \rho(Q^{-1}).\]

which is the second conclusion.

From the theoretical viewpoint, the above two theorems show lower and upper bounds on the average convergence rate. But in practice it is hard to apply the theoretical results since both spectral radii \(\rho(Q)\) and \(\rho(Q^{-1})\) are too difficult to calculate in most cases.
5.2 Computational Study

In this subsection, we propose a computational approach to illustrating the average convergence rate of randomised heuristics. Unlike the theoretical study, the calculation of the average convergence rate is rather simple in the computational study.

We run a randomised search heuristic $k$ times. Let $n(\Phi_t \in S_{\text{non}})$ denote the number of $\Phi_t$ (where $t = 0, 1, \cdots$) appearing in the non-optimal set for these $k$ runs. Then in practice, we will take

\[
\frac{-1}{t} \ln \frac{n(\Phi_t \in S_{\text{non}})}{k}
\]

as the average convergence rate.

**Example 4.** Consider RSH-I and RSH-II for solving the maximising problem

$$\max x^2, x \in \{0, \cdots, 100\}.$$

We run each algorithm for 100,000 times. The initial population is $\Phi_0 = 20$. If $n(\Phi_t \in S_{\text{non}}) \leq 10^{-5}$ happens, we don’t calculate the average convergence rate. It is due to the following reason: the event $n(\Phi_t \in S_{\text{non}}) \leq 10^{-5}$ is a small probability event. Computer simulation in 100,000 runs is not enough from the statistical viewpoint.

Figure 3 shows the average convergence rate of RSH-I is much higher than that of RSH-II. Initially the average convergence rate of both algorithms is 0. Then the average convergence rate of RSH-I increases from 0 to about 0.0009 quickly, but the average rate of RSH-II increases from 0 to about 0.0004 slowly.

![Figure 3: The average convergence rate of RSH-I and RSH-II for maximising $x^2$.](image)

The average convergence rate is different from the logarithmic progress rate, $\ln f_t$, used in some references (for example, see Figures 8 and 9 in [33]). Such a logarithmic rate may provide an intuitive description of the fitness change, but does not give a quantitative measure of the convergence rate itself. Let’s demonstrate this by the following example.

**Example 5.** Consider RSH-II for solving the following two problems,

$$\max x^2, \max = 10x^2, x \in \{0, 1, \cdots, 100\}.$$

We run the algorithm for 100,000 times. The initial population is $\Phi_0 = 20$. Figure 4 depicts that the logarithmic progress rate of RSH-II on the function $10x^2$ is larger than that on the function $x^2$. It is caused by the coefficient difference between the two fitnesses. The logarithmic progress rate is not a quantitative measure of the convergence rate.

6 Expected Hitting Times

6.1 Theoretical Study 1:: Fundamental Matrix

In this subsection, we define the expected hitting time and fundamental matrix. The first hitting time is the number of iterations to find an optimal solution for the first time, which is an important measure of the
Figure 4: The logarithmic progress rate \( \ln f_t \) of RSH-I for maximising \( x^2 \) and \( 10x^2 \).

performance of randomised search heuristics. Its formal definition is given as below.

**Definition 3.** Suppose the initial population \( \Phi_0 = X \). The mean number of iterations when a randomised search heuristic encounters an optimal solution for the first time is called the expected hitting time, denoted by \( h(X) \).

When we talk about the expected hitting time, we always assume that randomised search heuristics are convergent. Otherwise the expected hitting time is infinite, and that is out of our interest.

Let \((X_1, X_2, \cdots)\) represent all populations in the non-optimal set. Then the vector

\[ h = (h(X_1), h(X_2), \cdots)^T, \]

represents expected hitting times corresponding to all non-optimal populations.

In absorbing Markov chains, the fundamental matrix plays a crucial role which is defined as follows.

**Definition 4.** [13, Definition 11.3] For an absorbing Markov chain \( \{\Phi_t; t = 0, 1, \cdots\} \) with the transition matrix \( Q \), the matrix \( N = (I - Q)^{-1} \) is called the fundamental matrix.

Now we explain the meaning of the entry \( N(X, Y) \) of the fundamental matrix. Since the chain is convergent (i.e., \( \rho(Q) < 1 \)), then

\[ N = (I - Q)^{-1} = \sum_{t=0}^{+\infty} Q^t. \]

Rewriting the above equality in the entry form, we get

\[ N(X, Y) = \sum_{t=0}^{+\infty} P(\Phi_t = Y \mid \Phi_0 = X). \]

Therefore \( N(X, Y) \) is the mean number of the chain visiting \( Y \) when starting at \( X \) [13, Definition 11.3].

The hitting time vector \( h \) can be calculated by the fundamental matrix. According to Theorem 11.5 in [13], for an absorbing Markov chain \( \{\Phi_t; t = 0, 1, \cdots\} \), its expected hitting times equal to

\[ h = N1, \] (20)

where \( 1 \) is a column vector all of whose entries are 1.

However, it is difficult to apply the above result to the analysis of expected hitting time since it is impossible to calculate the fundamental matrix in most cases.
6.2 Theoretical Study 2: Average Drift Analysis

In this subsection, we present average drift analysis for bounding the expected hitting time, which is seldom investigated before. The first work to use less point-wise drift was [20]. Recently average drift analysis was applied to the runtime analysis of an EA for unimodal functions.

It is too difficult to calculate the expected hitting time through the fundamental matrix. Instead it is more realistic to obtain their lower and upper bounds on expected hitting time. Drift analysis was introduced in bounding the expected hitting time of randomised search heuristics [14, 16]. In drift analysis, \( d(X) \) is called a drift function if \( d(X) \geq 0 \) for any non-optimal state \( X \) and \( d(X) = 0 \) for any optimal state \( X \). Given a drift function \( d(X) \), drift represents the progress rate of moving towards the optima per iteration.

**Definition 5.** Drift at point \( X \) is defined by

\[
\Delta(X) := d(X) - \sum_{Y \in S_{\text{non}}} d(Y)P(X,Y).
\]

Let \( (X_1, X_2, \cdots) \) represent all populations in the non-optimal set and the vector

\[
d = (d(X_1), d(X_2), \cdots)^T
\]

represents the drift function values corresponding to each non-optimal state. The vector

\[
\Delta = (\Delta(X_1), \Delta(X_2), \cdots)^T
\]

represents the drift value corresponding to each non-optimal state.

The drift \( \Delta(X) \) is determined by a single state \( X \). So it is called point-wise drift. Now we introduce average drift which is the average of \( \Delta(X) \) over the probability distribution of \( \Phi_t = X \).

**Definition 6.** Average drift at the \( t \)-iteration is

\[
\bar{\Delta}_t := \sum_{X \in S_{\text{non}}} \Delta(X) \frac{P(\Phi_t = X)}{P(\Phi_t \in S_{\text{non}})}
\]  

Let \( h(\Phi_0) \) denote the expected hitting time when the initial population is \( \Phi_0 \), that is,

\[
h(\Phi_0) = \sum_{X \in S_{\text{non}}} h(X)P(\Phi_0 = X).
\]

Let \( d(\Phi_0) \) denote the expected drift function when the initial population is \( \Phi_0 \), that is,

\[
d(\Phi_0) = \sum_{X \in S_{\text{non}}} d(X)P(\Phi_0 = X).
\]

The following average drift theorem is for upper-bounding the expected hitting time.

**Theorem 4.** Suppose a randomised search heuristic is convergent. If for any \( t \geq 0 \), the average drift \( \bar{\Delta}_t \geq 1 \), then the expected hitting time \( h(\Phi_0) \) is upper-bounded by \( d(\Phi_0) \).

**Proof.** Recall that the 1-norm equals to

\[
\| q_t \|_1 = P(\Phi_t \in S_{\text{non}}),
\]

then the average drift can be rewritten in an equivalent vector form:

\[
\bar{\Delta}_t = \frac{q_t^T}{\| q_t \|_1} (I - Q)d.
\]

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\(^6\) Jun He, Tianshi Chen, Xin Yao: Average Drift Analysis and its Application. CoRR abs/1308.3080 (2013)
The condition that $\bar{\Delta}_t \geq 1$ can be rewritten in an equivalent vector form,

$$\frac{q_t^T}{\|q_t^T\|_1} (I - Q)d \geq 1.$$ 

It follows

$$q_t^T (I - Q)d \geq \|q_t^T\|_1,$$

then from $\|q_t^T\|_1 = q_t^T 1$, it follows

$$q_t^T (I - Q)d \geq q_t^T 1.$$ (23)

From the matrix iteration $q_t^T = q_0^T Q^t$, it follows

$$q_0^T Q^t (I - Q)d \geq q_0^T Q^t 1,$$

Equivalently

$$q_0^T (Q^t - Q^{t+1}) d \geq q_0^T Q^{t+1} 1,$$

Now summing $t$ from 0 to $k$, we get

$$\sum_{t=0}^{k} q_0^T (Q^t - Q^{t+1}) d \geq \sum_{t=0}^{k} q_0^T Q^{t+1} 1,$$

and simplifying both sides, it follows

$$q_0^T d - q_0^T Q^{k+1} d \geq q_0^T \left( \sum_{t=0}^{k} Q^t \right) 1.$$ (24)

Due to $\rho(Q) < 1$, the following two limits exist,

$$\lim_{k \to +\infty} Q^{k+1} = 0,$$

$$\lim_{k \to +\infty} \sum_{t=0}^{k} Q^t = (I - Q)^{-1}.$$ 

Thus when $k \to +\infty$, (24) becomes

$$q_0^T d \geq q_0^T (I - Q)^{-1} 1.$$

Recalling that $h = N1 = (I - Q)^{-1} 1$, we have

$$q_0^T d \geq q_0^T h.$$ 

which proves the conclusion.

Similarly we can establish an average drift theorem for lower-bounding the expected hitting time. Its proof is almost the same as that for the above theorem. We omit the proof of theorem.

**Theorem 5.** If for any iteration $t \geq 0$, the average drift $\bar{\Delta}_t \leq 1$, then the expected hitting time $h(\Phi_0)$ is lower-bounded by $d(\Phi_0)$.

Previous point-wise drift theorems [18, Theorems 2 and 3] are direct corollaries of current average drift theorems.

**Corollary 1.** If for any non-optimal population $X$, its drift $\Delta(X) \geq 1$, then the expected hitting time $h(X) \leq d(X)$.

**Corollary 2.** If for any non-optimal population $X$, its drift $\Delta(X) \leq 1$, then the expected hitting time $h(X) \geq d(X)$.

In point-wise drift theorems, its requirement is that the drift is not less than 1 (or not more than 1) for all non-optimal states. In average drift theorems, the condition is replaced by that average drift is not less than 1 (or not more than 1). Hence average drift analysis is more powerful than point-wise drift analysis.
6.3 Theoretical Study 3: Backward Drift Analysis

In this subsection, we present novel backward drift analysis, which was never discussed before. We call the drift defined in the previous subsection forward drift in order to distinguish it from the backward drift introduced in the current subsection. Forward and backward drift analysis can be regarded as a dual pair.

Starting from the fundamental matrix, we already know that the vector $h = N1$ represents all expected hitting times in the non-optimal set. Similarly the vector $s^T := 1^T N$

gives another type of important times for randomised search heuristics. Now we explain the intuitive meaning of the vector $s$. Notice that the entry

$s(Y) = \sum_{X \in S_{\text{non}}} N(X, Y)$,

and recall that $N(X, Y)$ is the expected number of that the Markov chain visits $Y$ when starting at $X$, then $s(Y)$ is the sum of the expected number of visiting state $Y$ when starting from all non-optimal states. We call $s(Y)$ the expected staying time in non-optimal state $Y$.

The expected hitting time and expected staying time have the following relationship.

**Theorem 6.** Let $h(X)$ be the expected hitting time from non-optimal population $X$ and $s(Y)$ the expected staying time in non-optimal population $Y$. Then

$$\sum_{X \in S_{\text{non}}} h(X) = \sum_{Y \in S_{\text{non}}} s(Y).$$

**Proof.** From the equalities

$$\sum_{X \in S_{\text{non}}} h(X) = 1^T N1,$n
$$\sum_{X \in S_{\text{non}}} s(X) = 1^T N1,$n

we draw the conclusion. $\square$

The above theorem implies that the expected hitting time equals to the expected staying time when the initial population is chosen at uniformly random.

Next we establish backward drift analysis for bounding the expected staying time. Like forward drift analysis, a drift function is used in backward drift analysis. $d(Y)$ is called a drift function if $d(Y) \geq 0$ for any non-optimal state $Y$ and $d(Y) = 0$ for any optimal state $Y$.

**Definition 7.** Let $d(Y)$ be a drift function. For a non-optimal population $Y$, the backward forward drift is

$$\nabla(Y) := d(Y) - \sum_{X \in S_{\text{non}}} d(X) P(X, Y).$$

Backward drift is to measure the move from $Y$ to $X$ (backward). This is different from forward drift

$$\Delta(X) := d(X) - \sum_{Y \in S_{\text{non}}} d(Y) P(X, Y).$$

which is to measure the move from $X$ to $Y$ (forward).

The following backward drift theorem is used for upper-bounding the staying time.

**Theorem 7.** If for any non-optimal population $Y$, its backward drift $\nabla(Y) \geq 1$, then the staying time $s(Y) \leq d(Y)$. 

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Proof. Let \((Y_1, Y_2, \cdots)\) represents all non-optimal populations and the vector
\[
\nabla^T = (\nabla(Y_1), \nabla(Y_2), \cdots)
\]
represents their drift function values respectively. Then from the definition, \(\nabla^T\) can be rewritten in the vector form as follows:
\[
\nabla^T := d^T (I - Q).
\]
(25)
The condition that \(\nabla(X) \geq 1\) is rewritten in a vector form \(d^T (I - Q) \geq 1^T\), and it follows \(d^T (I - Q) - 1^T \geq 0^T\).

Since the fundamental matrix \(N\) is non-negative, then
\[
(d^T (I - Q) - 1^T) N \geq 0^T,
\]
Since \(N = (I - Q)^{-1}\), so it follows \(d^T - 1^T N \geq 0^T\), and \(s^T \leq d^T\) which proves the conclusion.

Similarly we can establish a backward drift theorem for lower-bounding the staying time.

**Theorem 8.** If for any non-optimal population \(X\), its backward drift \(\nabla(X) \leq 1\), then the staying time satisfies \(s(X) \geq d(X)\).

Backward drift analysis provides an alternative way of bounding the expected hitting time when the initial population is chosen at uniformly random. It is possible to establish average backward drift analysis similar to average forward drift analysis. We will not discuss it in the detail.

### 6.4 Case Studies

In this subsection, we demonstrate how average drift analysis and backward drift analysis are applied to the estimation of the expected hitting time. There are three steps when applying drift analysis. First, choose an appropriate drift function; then estimate drift; finally, obtain a bound on the expected hitting time or staying time.

The first example is to show that average drift theorems work well but point-wise drift theorems are not applicable.

**Example 6.** Consider RSH-I for the maximizing problem
\[
\max x^2, \quad x \in \{0, 1, \cdots, 100\}.
\]
Choose the drift function as follows
\[
d(x) = \begin{cases}
100 \times 101 \times (100 - x), & \text{if } 1 \leq x \leq 99, \\
100 \times 101 \times d(x + 1), & \text{if } x = 0.
\end{cases}
\]
Calculate the drift \(\Delta(x)\). For \(1 \leq x \leq 99\),
\[
\Delta(x) = d(x) - 0.99d(x) - 0.01d(x + 1) = \frac{101}{99},
\]
\[
\Delta(0) = d(0) - 0.99d(0) - 0.01d(1) = 0.
\]
Notice that \(\Delta(0) = 0\), thus point-wise drift theorems cannot be applied here.
However, average drift theorems work well. Assume that the initial population \(\Phi_0\) is chosen at uniformly random, that is, \(P(\Phi_0 = x) = 1/101\). The average forward drift is
\[
\bar{\Delta}_0 = \left( \frac{1}{101} \Delta(0) + \frac{1}{101} \sum_{x=0}^{99} \Delta(x) \right) = 1.
\]
Since RSH-I adopts elitist selection, so that if initial population $\Phi_0 = x$ is not at state 0, then for any $t \geq 0$, its offspring $\Phi_t$ never returns to state 0. Thus the average forward drift is not less than

$$\bar{\Delta}_t = \left( \frac{1}{101} \Delta(0) + \frac{1}{101} \sum_{x=0}^{99} \Delta(x) \right) = 1.$$  

According to Theorem 4, the expected hitting time is not more than

$$\frac{1}{101} \sum_{x=0}^{99} d(x) = 5000.$$

The second example is to show that we can derive the same conclusion using backward drift analysis.

**Example 7.** Still consider RSH-I for the maximizing problem, 

$$\max x^2, \quad x \in \{0, 1, \cdots, 100\}.$$ 

Choose the drift function as follow 

$$d(x) = 100(x + 1), \quad 0 \leq x \leq 99,$$

Calculate the backward drift $\nabla(x)$. For $1 \leq x \leq 99$,

$$\nabla(x) = d(x) - 0.99d(x) - 0.01d(x - 1) = 1, \quad \nabla(0) = d(0) - 0.99d(0) = 1.$$ 

According to Theorems 7 and 8, the staying time 

$$s(x) = d(x) = 100(x + 1).$$ 

Furthermore if the initial population is chosen at uniformly random, then according to Theorem 6, the expected hitting time equals to 

$$\frac{1}{101} \sum_{x=0}^{99} s(x) = \frac{1}{101} \sum_{x=0}^{99} 100(x + 1) = 5000.$$ 

The result is the same as that in the first example by applying average drift analysis.

### 6.5 Computational Study

In this subsection, we illustrate a computational approach to the calculation of the expected hitting time.

In the computational study, we runs a randomised search heuristic for $k$ times. Let $\tau_i(X)$ be the first hitting time for the $i$-th run during these $k$ runs.

From the law of large numbers, the expected hitting time $h(x)$ is approximated by the average 

$$\frac{1}{k} \sum_{i=1}^{k} \tau_i(X), \quad \text{when } k \to +\infty. \quad (26)$$

The above average value is taken as the expected hitting time $h(X)$ in the computational study.

Sometimes it is easy to study the expected hitting time through the computational study.

**Example 8.** Consider RSH-I and RSH-II for solving the maximization problem 

$$\max x^2, \quad x \in \{0, 1, \cdots, 100\}.$$ 

We run each algorithm for 100,000 times. The initial population is $\Phi_0 = 20$. Figure 4 shows that the expected hitting time of RSH-II is about 16000, which is twice as long as that of RSH-I, about 8000.
However, sometimes the calculation of the expected hitting time needs an extremely long computation time.

**Example 9.** Consider RSH-II for solving the maximization problem

$$\max (x - 49)^2, \quad x \in \{0, 1, \ldots, 100\}.$$  

We run each algorithm for 100,000 times. We found that RSH-II always got stuck at the local optimum 0. Even for the simple problem, it seems not easy to make a computational study of the expected hitting time.

**7 Conclusions and Future Work**

A unified Markov chain approach has been proposed for studying the convergence, convergence rate and expected hitting time of randomised search heuristics in this paper. The core of the approach is to model randomised search heuristics by absorbing Markov chains and then to study the chain based on matrix iteration analysis. A novelty in the analysis is that the vector 1-norm is used to represent the probability of a population in the non-optimal solution set. It plays the role of the distance between a population and the optimal solution set. All theoretical results are proven in a unified manner.

The results of the paper are summarised as follow: First, Theorem 1 establishes a sufficient and necessary condition of convergence in distribution. The theorem states a randomised search heuristic is convergent if and only if the algorithm can make an improvement in finite iterations suppose the current solution is not optimal.

Then the average convergence rate is introduced, which refers to the average reduction factor of the probability of a population in the non-optimal set per iteration in terms of the logarithmic mean. Theorems 2 and 3 provide lower and upper bounds on the average convergence rate.

Finally, two new types of drift analysis, average drift analysis and backward drift analysis, are proposed for analysing the expected hitting time. Theorems 4 and 5 state that the expected hitting time can be bounded by a drift function and related average drift. Theorem 6 reveals that the expected hitting time and expected staying time are equal if the initial population is chosen at uniformly random. Theorems 7 and 8 state that the expected staying time can be bounded by a drift function and related backward drift.

Besides the theoretical study, computation approaches are also presented to study the convergence, average convergence rate and expected hitting time.

Comparing computational and theoretical studies, we see none of them are perfect. The computational study may provide an intuitive description of randomised search heuristics’ behaviour, but it belongs to a posterior and case study. On the other hand, the theoretical study belongs to a prior and general study. Theoretical results may provide some understanding of randomised search heuristics’ ability. But it is still too hard to obtain an exact value of the expected hitting time or average convergence rate.

There is a gap between the theoretical and computational studies. Our future work is to improve theoretical tools, to apply them to different types of randomised search heuristics and to study their convergence, convergence rate and expected hitting time.
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