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Bat Algorithm application for estimating Super Pairwise Alignment parameters on similarity analysis between virus protein sequences

Dinita Rahmalia[1], Teguh Herlambang[2]
[1]Universitas Islam Darul Ulum, Jalan Airlangga 3 Sukodadi, Lamongan, Indonesia
[2]Universitas Nahdlatul Ulama Surabaya, Jalan Jemursari 59, Surabaya, Indonesia

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ABSTRACT

Either virus or bacteria could cause many diseases, and they can mutate to form a new disease. Sequence alignment is a method used in the researches of various diseases. In this research, we took a case study of the dengue virus and Zika virus. The alignment process of two virus sequences would be used to determine the similarity between the mutated virus and the original virus. Super Pairwise Alignment (SPA) is the method applied in bioinformatics for aligning two virus sequences. Because the similarity score was affected on SPA-parameters, in these research we would apply meta-heuristic method, such as Bat Algorithm (BA) algorithm for optimizing SPA-parameters which can maximize similarity score. BA was the optimization method which was resemble by the action of bats in using sonar called echolocation to detect prey, avoid obstacles. From the BA simulations, we obtain optimum SPA-parameters in approaching which can result maximum similarity score between two aligned each of dengue virus and zika virus protein sequences.

Dinita Rahmalia,
Universitas Islam Darul Ulum, Jalan Airlangga 3 Sukodadi, Lamongan, Indonesia
Email: dinitarahmalia@gmail.com

1. INTRODUCTION

Either virus or bacteria can cause many diseases and they can mutate so that they could form the new disease. Mutations can create the growth or the death of cells, so that new disease is formed. Sequence alignment is the method so that it can be used to research various of disease whether in determining the variance, origin or epidemics development.

In this research, case study of dengue virus and zika virus will be taken as example. Zika virus has been found in 1947 in monkey and then it is identified in human in 1952 in Africa. *Aedes* mosquito can cause zika disease through bite with the symptoms are resemble to dengue fever [1]. Based on previous research, zika virus is mutation from dengue virus. In Indonesia, there are four types of dengue virus namely dengue virus-1, dengue virus-2, dengue virus-3 and dengue virus-4 [2]. In this research, each dengue virus protein sequence will be compared by zika virus protein sequence to be analyzed the similarity. For determining the similarity between mutated virus and the original virus, the alignment process of two virus sequences will be used. Super Pairwise Alignment (SPA) was the method in bioinformatics applied for aligning two virus sequences [3].

SPA-parameters selection is often applied by trial and error [4]. Because the similarity score is affected on SPA-parameters, the problems of this research are how we can estimate and optimize SPA-parameters maximizing similarity score between dengue virus and zika virus, so that the purpose of this research is applying meta-heuristic method, such as Bat Algorithm (BA) algorithm to estimate and optimize SPA-parameters which can maximize similarity score. In previous research, parameter estimations using heuristic method have been applied in forecasting [5], control problem applied in epidemics [6], and control proble applied in transportation [7]. In particular researches, SPA-parameters have also been optimized by Particle Swarm Optimization in dengue virus [8] and Artificial Bee Colony in mutation of zika virus [9]. In this research, we will optimize SPA parameters between two different disease, i.e. dengue virus and zika virus protein sequence.

Bat Algorithm (BA) was discovered by Xin She Yang in 2010. The bats use sonar called echolocation for locating in the dark, detect prey, and avoid obstacles. In the BA, there are local solution among the selected best solution based on loudness and pulse rates [10][11]. There are many researches about BA applications such as optimization problem by modified BA [12], transport network design problem [13], Travel Salesman Problem (TSP) [14], Vehicle Routing Problem (VRP) with time windows [15], flowshop scheduling problem [16], jobshop scheduling problem [17], goal programming on multiobjective function [18], image classification [19], designing fuzzy controller [20], and designing PID controller [21].

BA simulations have been applied between each dengue virus and zika virus. We obtain optimum SPA parameters in approaching which can result maximum similarity score between two aligned each of dengue virus and zika virus protein sequences. Moreover, we can obtain the position and length of sequence unit which is occured insertions and deletions.

2. RESEARCH METHOD

2.1. Biological Sequences

There are terms in the study of biological sequences like DNA, RNA, and protein sequences. DNA (deoxyribonucleic acid) molecule is two strands of nucleotides twisted. Protein-coding genes are for producing proteins. They are linear polymers of twenty amino acids connected by peptide bond. RNA (ribonucleic acid) is single-stranded and related to DNA [22].

In DNA, RNA or protein sequence, their structure consists of the nucleotides component. Generally the following description of a biological sequence is as follows

$$\bar{A} = (a_1, a_2, ..., a_{n_a}), \bar{B} = (b_1, b_2, ..., b_{n_b}), \bar{C} = (c_1, c_2, ..., c_{n_c})$$

With $\hat{A}, \hat{B}$ are the sequences, and a_i, b_i are the units of the sequence, at position i

$\hat{A}, \hat{B}$ are DNA when the unit of the sequence are $\{A, C, G, T\}$

$\hat{A}, \hat{B}$ are RNA when the unit of the sequence are $\{A, C, G, U\}$

$\hat{A}, \hat{B}$ are protein sequences when the unit of the sequences are *{A, C, D, E, F, G, H, I, K, L, M, N, P, Q, R, S, T, V, W, Y}*

2.2. Sequence Alignment

If the sequence has relatedness to the its pair, then two sequences are homologous. The step for inferring homology is determining the sequence similarity. To determine the similarity, we have to align them properly. For example, the two nucletides sequences, *X* and *Y*

$$X : TACCAGT$$
$$Y : CCCGTAA$$

If there are gaps, there are many possible alignment either case 1 or case 2 so that we must choose better alignment.

Case 1 :

$$X : TACCAGT - -$$
$$Y : C - CC - GTAA$$

Case 2 :

$$X : TACCAGT - -$$
$$Y : - - CCCGTAA$$

2.3. The Type of Mutation

In molecular biology, the mutation of sequence A will change sequence A into sequence B. There are four types of the mutations [3]:

Type I : The mutation by segment changing to another.
Type II : The mutation by segment permuting its position.
Type III : The mutation by inserting new segment into sequence.
Type IV : The mutation by deleting the segment from sequence.

In this research, we restrict the problem only using type III and type IV mutations.

2.4. Comparison Two Sequences

The sequence alignment problem is finding the structure so that the sequences have difference or similarity. It is noted in penalty matrix *W* whose the elements of penalty matrix can be seen in equation (1).

$$w(a_i, b_i) = \begin{cases} 0, & if\ a_i = b_i \\ 1, & otherwise \end{cases}, i = 1,2,\dots,n \quad (1)$$

Let two sequences $(A = (a_1, a_2, ..., a_n))$ and $(B = (b_1, b_2, ..., b_n))$. Sliding Window Function of sequence A and sequence B can be seen in equation (2) with *i* is the sequence unit initial number of sequence A and *j* is the sequence unit initial number of sequence B, and *n* is the length of sequence.

$$w(A, B, i, j, n) = \frac{1}{n}\sum_{k=1}^{n} w(a_{i+k}, b_{j+k}) \quad (2)$$

2.5. Shifting Mutation Modulus Structure

If sequence A mutate into sequence B by shifting mutations, then it can be constructed as in equation (3).

$$A = (a_1, ..., a_{n_a}) \overset{III}{\rightarrow} C = (c_1, ..., c_{n_c}) \overset{IV}{\rightarrow} B = (b_1, ..., b_{n_b}) \quad (3)$$

By shifting mutation T, and $A \overset{T}{\rightarrow} B$, the mutation operations applied is as follows :

$$T = \{(i_k, l_k), k = 1, 2, ..., k_a\} \quad (4)$$

The k_a in T is the shifting mutations total of sequence A. The pair (i_k, l_k) consist of i_k is the shifting mutation position, and l_k is the the type and length of the k-th shifting mutation. If $l_k > 0$, it is the type III mutation and if $l_k < 0$, it is the type IV mutation. $|l_k|$ is the length of the deleted or inserted segment [3].

2.6. Super Pairwise Alignment (SPA) Algorithm

SPA algorithm is used for computing similarity between two sequences. Let (A, B) are two sequences with sequence A mutates into sequence B. SPA works by partiting the sequence and analyzing the similarity on the partited sequence respectively. The parameters of SPA are (n, θ, ϕ) with interval are $n > 0$; $0.3 \le \theta \le 0.4; \theta < \phi \le 1$ [3]. The parameters of SPA consist of the length of partited sequence unit n, the threshold where two partited sequences have almost been similar θ, the threshold where two partited sequences have not been similar yet ϕ , so that they may be mutated and require shifting process either insertion or deletion.

1. Estimate the first mutation position $\hat{i}_1$ in T

   Initialization $i = j = 0$ and compute $(w(A, B, i, j, n))$ based on equation (2).

   a. If $w(A, B, i, j, n) \ge \phi$

      $\hat{i}_1 = 0$

      End

   b. If $w(A, B, i, j, n) < \phi$

      Let $i = j = (k_1(n - \tau))$ with k_1 is the integer.

      Compute $(w(A, B, i, j, n))$.

      If $w(A, B, i, j, n) < \phi$, do the steps 1(b) by updating $k \leftarrow k + 1$ until $w(A, B, i, j, n) \ge \phi$, and store the value of i and j as $\hat{i}_1$

      End

2. Based on the estimation $\hat{i}_1$, estimate $\hat{l}_1$ using this procedure

   $w(A, B, \hat{i}_1 + l, \hat{i}_1, n)$, $w(A, B, \hat{i}_1, \hat{i}_1 + l, n)$, $l = 1, 2, 3, ..., l_{\max}$

   a. If $w(A, B, \hat{i}_1 + l, \hat{i}_1, n) \le \theta$, then $\hat{l}_1 = -l$. This means occuring deletion l segments from sequence A to sequence B.

b. If $w(A,B,\hat{i}_1,\hat{i}_1+l,n)\le\theta$, then $\hat{l}_1=l$. This means occuring insertion l segments from sequence A to sequence B.

Then, local mutation mode $T_1=\{(i_1,l_1)\}$, and locally uniform alignment (C_1,D_1) are formed.

3. Repeat its process until k_0
4. Compute objective :

Similarity score between whole aligned sequence C_{k_0} and sequence D_{k_0} in equation (5)

$$s(C_{k_0},D_{k_0})=\frac{1}{N}\sum_{j=1}^{N}s(c_j,d_j) \tag{5}$$

whose the element

$$s(c_j,d_j)=\begin{cases}1, & if\ c_j=d_j\\ 0, & otherwise\end{cases}$$

2.7. Bat Algorithm

Bat Algorithm (BA) was discovered by Xin She Yang in 2010. The bats use sonar named echolocation for locating in the dark, detect prey, and avoid obstacles. The action of bats are as follows [10],[11]:

1. Echolocation is applied by bats for sensing the food, distances, barries, and prey.
2. Bat flies randomly in position x_i with velocity v_i by various wavelength, fixed frequency $f_{\min}$, and loudness A^0 for searching the prey. They adapt the pulse rate.
3. The loudness changes from the large positive A^0 to the small $A_{\min}$

Based on action of bats, the BA applied to optimization model of SPA can be constructed as follows :

Suppose objective function $f:R^D\to R$ with D is the search space dimension.

In initialization, build the initial solutions randomly $x_{ij}, i=1..maxpop, j=1..D$ and compute the fitness $f(x_{ij}), i=1..maxpop, j=1..D$. In BA applied to optimization model of SPA, let $X=(n,\theta,\phi)$ as decision variable with objective in equation (5) for maximum similarity score.

1. Initialize the population of bat position x_i, $i=1,2,...,maxpop$, velocity v_i, $i=1,2,...,maxpop$, and pulse frequency f_i, $i=1,2,...,maxpop$
2. Initialize loudness A_i and pulse rates r_i
3. Do procedure as follows :

for $t=1:t\max$

for $i=1:maxpop$

$$f_i=f_{\min}+(f_{\max}-f_{\min})\beta\ ,\ \ \beta\sim U(0,1) \tag{6}$$

$$v_i^t=v_i^{t-1}+(x_i^t-x^*)f_i \tag{7}$$

$$x_i^t=x_i^{t-1}+v_i^t \tag{8}$$

end

if $(rand>r_i)$

- Generate local solution among the selected best solution

$$x_{new}=x_{old}+\in A^t, \text{ with } \in\sim U(-1,1) \tag{9}$$

end

if $(rand>A_i\ \&\ f(x_i)>f(x^*))$

- Keep new solution x_i
- Reduce A_i and increase r_i and so that $A_i^t\to 0, r_i^t\to r_i^0$

$$r_i^{t+1}=r_i^0(1-\exp(-\gamma t)), \text{ with } \gamma>0 \tag{10}$$

$$A_i^{t+1} = \alpha A_i^t, \text{ with } 0 < \alpha < 1 \quad (11)$$

end

Find current best x^*

end

3. RESULTS AND DISCUSSION

Based on previous research [1], zika virus is mutation from dengue virus. In Indonesia, there are four types of dengue virus namely dengue virus 1, dengue virus 2, dengue virus 3 and dengue virus 4. In this research, each dengue virus protein sequence will be compared by zika virus protein sequence to be analyzed the similarity. The source of data are from National Center for Biotechnology Information (NCBI) taken on May 2, 2019. The characteristics of dengue virus and zika virus protein data can be seen in Table 1, where each virus type has unique access code with length is the number of amino acids of virus protein sequences.

Table 1. Dengue virus and zika virus protein data.

Access Code	Virus Type	Length (bp)
AHG06327	Dengue virus-1	3392
AHG06364	Dengue virus-2	3391
AHG06376	Dengue virus-3	3390
AHG06382	Dengue virus-4	3387
AMK49492	Zika virus	3429

The samples of dengue virus protein sequences which have been obtained from NCBI can be seen in Figure 1(a-d) while zika virus protein sequences can be seen in Figure 2. In protein sequences, there are protein-coding genes. They are linear polymers of twenty amino acids connected by peptide bond [22], with amino acid codes can be seen in Table 2.

Table 2. Amino acid of protein sequences.

Code	Amino Acid
'A'	"Alanine"
'C'	"Cysteine"
'D'	"Aspartic acid"
'E'	"Glutamic acid"
'F'	"Phenylalanine"
'G'	"Glycine"
'H'	"Histidine"
'I'	"Isoleucine"
'K'	"Lysine"
'L'	"Leucine"
'M'	"Methionine"
'N'	"Asparagine"
'P'	"Proline"
'Q'	"Glutamine"
'R'	"Arginine"
'S'	"Serine"
'T'	"Threonine"
'V'	"Valine"
'W'	"Tryptophan"
'Y'	"Tyrosine"

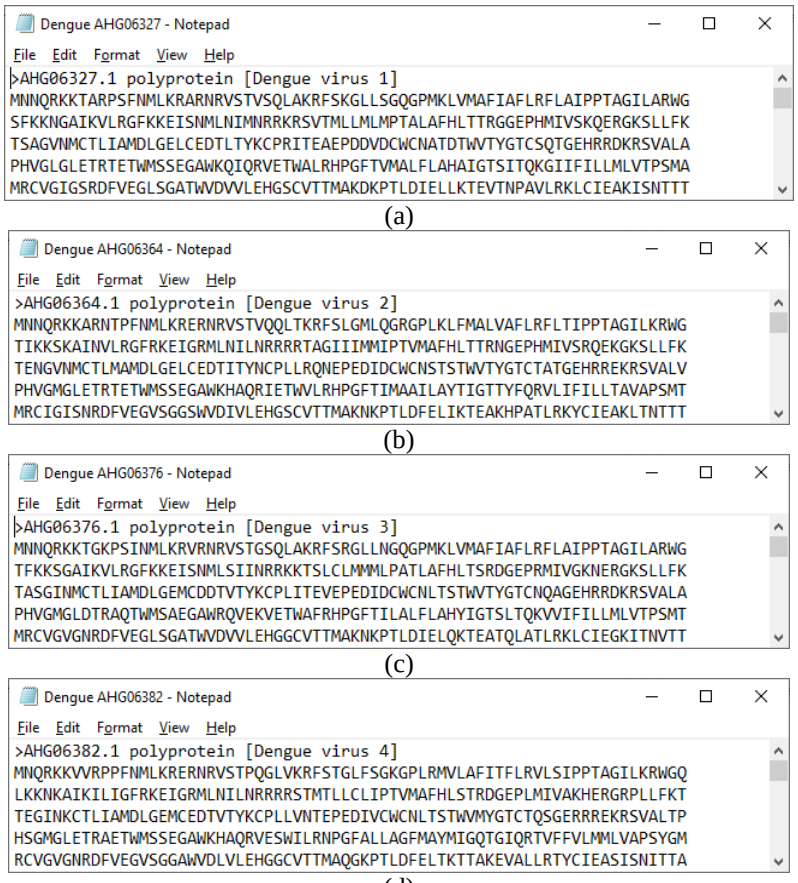


Fig. 1. The sample of dengue virus protein sequence (a) Dengue virus-1 (b) Dengue virus-2 (c) Dengue virus-3 (d) Dengue virus-4

Fig. 2. The sample of zika virus protein sequence

Bat Algorithm (BA) simulation is for finding SPA-parameters (n, θ, ϕ) which result maximum similarity score (excluding gaps) between two aligned dengue virus and zika virus protein sequences as objective. BA parameters used in each simulation are :

The number of population : 10
The maximum iteration : 50
The fixed Frequency : $f_{\min} = 0 \quad f_{\max} = 1$
The loudness : $A_0 = 10 \quad A_{\min} = 0$
The rate of pulse emission : $r_0 \in (0,1)$

Simulations are run by Matlab in Asus Laptop, CPU Intel 2 Core N3350, 2.4 GHz, Memory (RAM) 4 GB, HDD 500 GB, OS Windows 10.

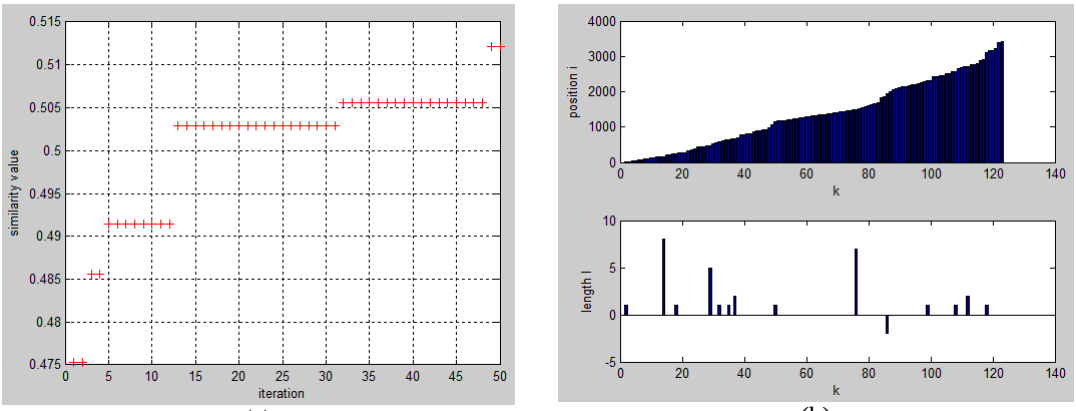
3.1. Similarity Analysis Between Dengue Virus 1 and Zika Virus

Figure 3(a) shows BA process of similarity score maximization of aligned dengue virus 1 and zika virus protein sequence. In the initial, bats fly randomly with the position as SPA-parameters with varying wavelength, a fixed frequency, and loudness for searching prey. In the optimization, the loudness decreases

and the pulse rate increases so that bat can find SPA-parameters with maximum score. The optimum SPA-parameters are $((n,\theta,\phi)=(13;0.3973;0.5126))$ with maximum similarity score based on equation (5) is 0.5121 or 51.21%. Because the similarity score is more than 25 %, we can declare that sequences are homologous (have similarity each other) [3].

Figure 3(b) shows the positions i_k and lengths l_k of optimum SPA-parameters. Optimum SPA-parameters result iteration $k=123$ when partition processes of whole sequences finish. From the graphs, positions i_k and lengths l_k can be seen. If $l_k>0$, insertion occurs (type III mutation), if $l_k<0$, deletion occurs (type IV mutation), and if $l_k=0$, mutation shifting is nothing.

As example, in iteration *k=14* in Figure 3(b), there are insertion l_k by 8 segments into zika virus protein sequence from dengue virus 1 in position 170. In iteration *k=86*, there are deletion l_k by 2 segments into zika virus protein sequence from dengue virus 1 in position 1936. When in Figure 3(b) does not show insertion or deletion, then there is no mutation shifting in the corresponding position i_k.



(a) (b)

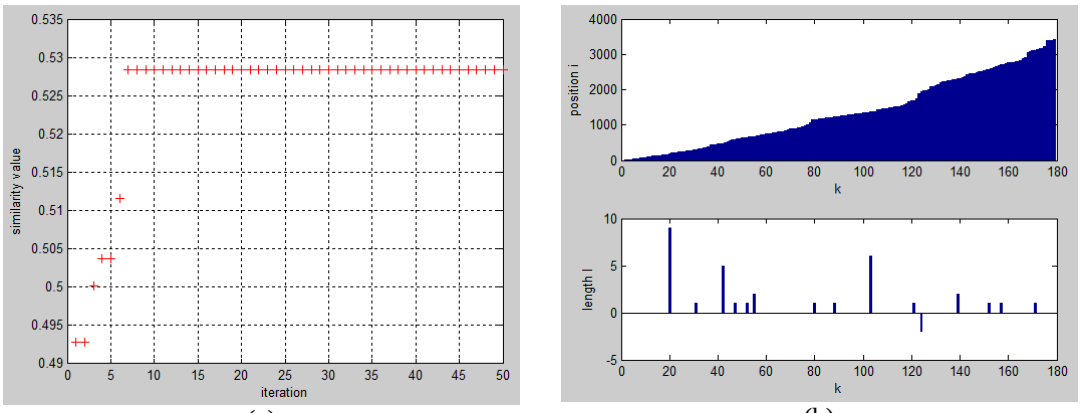
Fig. 3. Optimization process of aligned dengue virus 1 and zika virus protein sequences (a) BA optimization process (b) Lengths and positions of optimum SPA-parameters

3.2. Similarity Analysis Between Dengue Virus 2 and Zika Virus

Figure 4(a) shows BA process of similarity score maximization of aligned dengue virus 2 and zika virus protein sequence. In the initial, bats fly randomly with the position as SPA-parameters with varying wavelength, a fixed frequency, and loudness for searching prey. In the optimization, the loudness decreases and the pulse rate increases so that bat can find SPA-parameters with maximum score. The optimum SPA-parameters are $((n,\theta,\phi)=(9;0.3674;0.5348))$ with maximum similarity score based on equation (5) is 0.5285 or 52.85%. Because the similarity score is more than 25 %, we can declare that sequences are homologous (have similarity each other) [3].

Figure 4(b) shows the positions i_k and lengths l_k of optimum SPA-parameters. Optimum SPA-parameters result iteration $k=179$ when partition processes of whole sequences finish. From the graphs, positions i_k and lengths l_k can be seen. If $l_k>0$, insertion occurs (type III mutation), if $l_k<0$, deletion occurs (type IV mutation), and if $l_k=0$, mutation shifting is nothing.

As example, in iteration *k=20* in Figure 4(b), there are insertion l_k by 9 segments into zika virus protein sequence from dengue virus 2 in position 177. In iteration *k=124*, there are deletion l_k by 2 segments into zika virus protein sequence from dengue virus 2 in position 1686. When in Figure 4(b) does not show insertion or deletion, then there is no mutation shifting in the corresponding position i_k.



(a) (b)

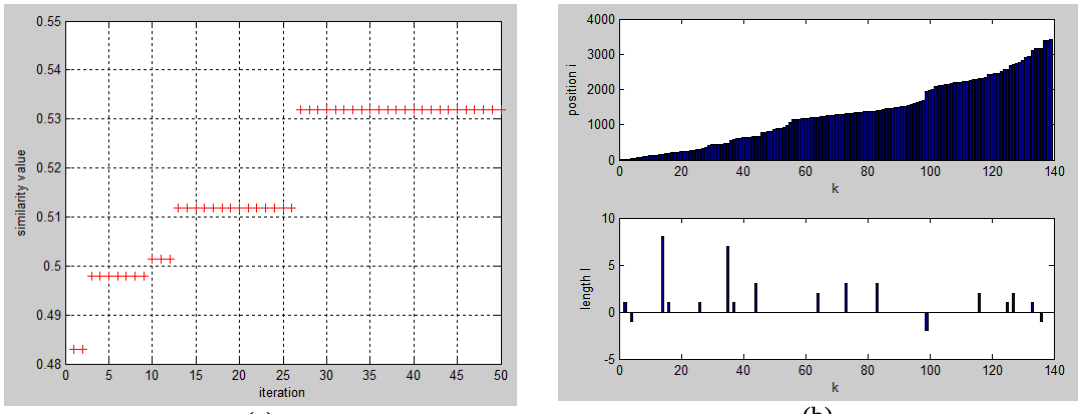
Fig. 4. Optimization process of aligned dengue virus 2 and zika virus protein sequences (a) BA optimization process (b) Lengths and positions of optimum SPA-parameters

3.3. Similarity Analysis Between Dengue Virus 3 and Zika Virus

Figure 5(a) shows BA process of similarity score maximization of aligned dengue virus 3 and zika virus protein sequence. In the initial, bats fly randomly with the position as SPA-parameters with varying wavelength, a fixed frequency, and loudness for searching prey. In the optimization, the loudness decreases and the pulse rate increases so that bat can find SPA-parameters with maximum score. The optimum SPA-parameters are $((n,\theta,\phi)=(9;0.3366;0.5604))$ with maximum similarity score based on equation (5) is 0.5319 or 53.19%. Because the similarity score is more than 25 %, we can declare that sequences are homologous (have similarity each other) [3].

Figure 5(b) shows the positions i_k and lengths l_k of optimum SPA-parameters. Optimum SPA-parameters result iteration $k=139$ when partition processes of whole sequences finish. From the graphs, positions i_k and lengths l_k can be seen. If $l_k>0$, insertion occurs (type III mutation), if $l_k<0$, deletion occurs (type IV mutation), and if $l_k=0$, mutation shifting is nothing.

As example, in iteration *k=14* in Figure 5(b), there are insertion l_k by 8 segments into zika virus protein sequence from dengue virus 3 in position 155. In iteration *k=99* in, there are deletion l_k by 2 segments into zika virus protein sequence from dengue virus 3 in position 1939. When in Figure 5(b) does not show insertion or deletion, then there is no mutation shifting in the corresponding position i_k.



(a) (b)

Fig. 5. Optimization process of aligned dengue virus 3 and zika virus protein sequences (a) BA optimization process (b) Lengths and positions of optimum SPA-parameters

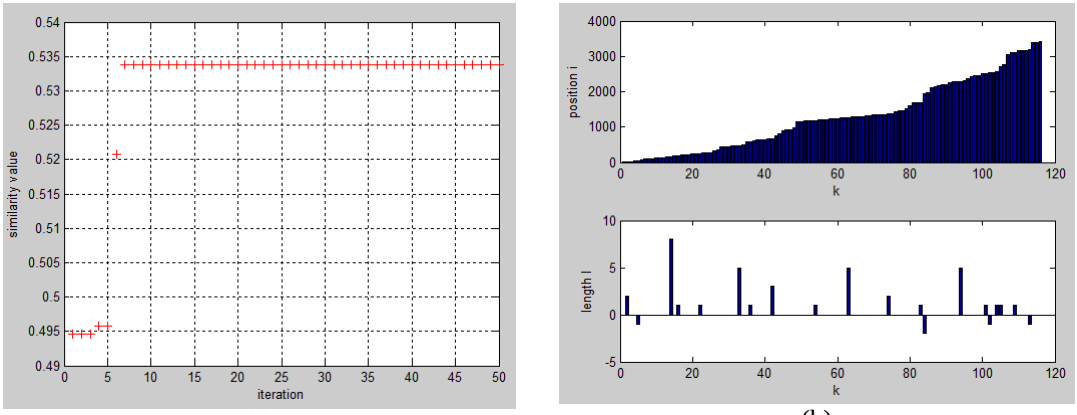
3.4. Similarity Analysis Between Dengue Virus 4 and Zika Virus

Figure 6(a) shows BA process of similarity score maximization of aligned dengue virus 4 and zika virus protein sequence. In the initial, bats fly randomly with the position as SPA-parameters with varying

wavelength, a fixed frequency, and loudness for searching prey. In the optimization, the loudness decreases and the pulse rate increases so that bat can find SPA-parameters with maximum score. The optimum SPA-parameters are $((n,\theta,\phi)=(8;0.3889;0.6267))$ with maximum similarity score based on equation (5) is 0.5338 or 53.38%. Because the similarity score is more than 25 %, we can declare that sequences are homologous (have similarity each other) [3].

Figure 6(b) shows the positions i_k and lengths l_k of optimum SPA-parameters. Optimum SPA-parameters result iteration $k=116$ when partition processes of whole sequences finish. From the graphs, positions i_k and lengths l_k can be seen. If $l_k>0$, insertion occurs (type III mutation), if $l_k<0$, deletion occurs (type IV mutation), and if $l_k=0$, mutation shifting is nothing.

As example, in iteration *k=14* in Figure 6(b), there are insertion l_k by 8 segments into zika virus protein sequence from dengue virus 4 in position 152. In iteration *k=84*, there are deletion l_k by 2 segments into zika virus protein sequence from dengue virus 4 in position 1942 (see Figure 6(b)). When in Figure 6(b) does not show insertion or deletion, then there is no mutation shifting in the corresponding position i_k.



(a) (b)

Fig. 6. Optimization process of aligned dengue virus 4 and zika virus protein sequences (a) BA optimization process (b) Lengths and positions of optimum SPA-parameters

4. CONCLUSION

Dengue virus protein sequence is the mutation from zika virus protein sequence, so that they are homologous sequence and they have similarity. For determining the similarity between mutated virus and the original virus, the alignment process of two virus sequences will be used. Super Pairwise Alignment (SPA) is the method in bioinformatics applied for aligning two virus sequences. In SPA, the similarity score is affected on SPA parameters. The SPA-parameters can be optimized by meta-heuristic method, such as Bat Algorithm (BA) from the action of bats. In the case study of dengue virus and zika virus protein, BA can find optimum SPA-parameters in approaching which can result maximum similarity score. Moreover, we can obtain the position and length of sequence unit which is occured insertions and deletions.The development of this research is optimization the similarity of more than two sequences (multiple sequences).

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BIOGRAPHY OF AUTHORS

Dinita Rahmalia, Lecturer of Mathematics Department. Universitas Islam Darul Ulum Lamongan. The research fields are optimization and operations research, control system, and data mining
Email : dinitarahmalia@gmail.com

Teguh Herlambang, Lecturer of Information System Department. Universitas Nahdlatul Ulama Surabaya. The research fields are applied mathematics, modelling, navigation and guidance
Email : teguh@unusa.ac.id