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Using intelligent optimization algorithms, determine the quality of the nitrogenous base substituted for the MT-ND5 gene sequence

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Abstract

This paper focuses on the application of intelligent optimization techniques in genetic engineering, using the MT-ND5 gene sequence as a case study to determine the specificity of nitrogenous base substitution. We used data from the NCBI database and analyzed it using smart optimization algorithms for the mathematical model of the objective function of the type of dynamic programming that comes from the hidden Markov chain to find the chance of getting a true sequence that is highest. We compared the results with the intelligent methods, demonstrating the effectiveness of these solutions in speeding up and enhancing the accuracy of the analysis through MATLAB simulations.

Key words and phrases: MT-ND5 gene, Ant colony optimization(ACO), Hidden Markov Model (HMM).

Mathematics Subject Classification (2010): 60J10, 92D20

1. Introduction

Identifying functions of gene sequences and determining the nitrogenous bases occurring in gene sequences accurately are very important since gene sequences bear individual details regarding creatures. Sample clustering can be made by pairwise comparisons of gene sequences by simplifying homolog gene comparisons in related species using molecular profiling. A Swarm Algorithm or Swarm Intelligence is used to eliminate the hard processing efforts and the problems such as local minima, slow convergence, and single-solution focus that standard optimization algorithms have in identifying the nitrogenous base in gene sequences [1]. We can pair the MT-ND5 gene sequence, which is

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the subject of our study here, and it is located in the mitochondrial genome. It has a crucial function particularly in the respiratory chain and in the production of ATP molecules. We can say Swarm Algorithms are a straightforward, simple application to the Penetrable Ellipsoids Model controller, neural network optimization, and interconnection weights of a fixed topology of neuro-fuzzy system problems; and widely used, the simple method that shows good results [2].

The main advantage of swarm algorithms is that they have low computational costs. For this reason, the long execution times of complex engineering problems are reduced by means of SA methods, providing faster response times than traditional optimization methods. The Swarm Algorithm also provides better quality performance than other optimization algorithms. SA can produce good results with less computational cost and faster convergence, providing a great advantage over classical optimization algorithms and genetic programming algorithms used extensively in gene studies. We aim to have the transgenic MT-ND5 gene, the first transgenic gene of microalgae. With swarm algorithms, we offer an alternative to modelling reliable and functional genetic sequences that are of great importance by providing an example for determining the base ratio. Thus, believing that the work has introduced noteworthy contributions, and a guide for various sections of the scientific field has been carried out [3].

1.1. Background and Significance

Biologically, transfer nucleic acid (TNA) plays the role of coenzyme for peptidyl transferase. Among them, mitochondria have strong specificity for producing 23s rRNA and 5s rRNA. When the structure and sequences of nucleotides meet the same conditions and can be used to organize mixed nucleotides with nucleotides in the same withdrawal, they can sometimes only figure out the target of nucleic acid. Determining the purpose of disease research is crucial. At the same time, developing convenient, fast, efficient, and effective technology and equipment to replace traditional manual work is also our primary goal. In addition to studying the structure of nucleic acids and enzyme bases, studying bases is one of the most useful methods for studying problems such as species identification and disease. Currently, computational-oriented studies model these issues as complex mathematical problems and attempt to solve them using intelligent technologies such as swarm intelligence [4].

As the biological spectrum and computer technology continue to advance, biological databases are now capable of storing vast amounts of nucleic acid and protein biology data. At the same time, bioinformatic spiders are beginning to digitize molecular biology signals and information. The computer converts nucleic acid signals into digital signals to speed up its search process. Researchers input digital signals and data that adhere to international standards. The capacity to perform significant functions, like altering gene defects and influencing epigenetics, is crucial. Acrylic DNA binds to sugar and utilizes the RAM size mode to interact with mRNA, a crucial tool for gene replication and expression. The two competing methods, CreateMap and Facetsmap, distinguish this approach from other multiple inference methods [5].

1.2. Research Objectives

The primary purpose of this study was to determine the possibility of using swarm algorithms in place of other optimization methods in this specific application. Secondly, the difficulties of the chosen application were to illustrate the reason for insufficient information to suggest a more general determination of bioinformatics. The objective of this study was, in general, to prove the potential of Swarm Intelligence, which has already been proven to be a good choice for the general optimization issues of bioinformatics, but which has not been tested in this specific application before. The application of Swarm Intelligence has two main layers. The first layer is directed to make the substitution of the nucleotide correctly from the raw data without any preprocessing. The second layer is about the determination of the substituted nitrogenous bases. The idea under the determination of substitution

of nitrogenous bases is to define the closest neighbour of the original solution, setting restriction conditions.

It was also found that the deterministic model prediction of the binding scores was enough for a higher level of coarse-graining. Finally, it was shown that the presented DNA scaling function generated two-fold better members compared to similar models in terms of recombination and articulation rates. Metaheuristics are proposed for the fine-grained redundancy reduction on formed particles, and they had better performance.

2. Overview of MT-ND5 Gene and Nitrogenous Bases

MT-ND5 (ND5) is the gene sequence in the mitochondrial genome of humans. It plays a vital role in forming a multisubunit protein complex with other NADH dehydrogenase genes to form complex I, which widely exists in eukaryotes from lower to higher organisms. Substituted nitrogenous bases are the key material basis of gene expression in organisms, which play an important role in genetic information and energy metabolism. More and more studies show that there always exist some variations in nitrogenous bases in the MT-ND5 gene sequence. The SNP, haplotype, typical, or special mutation can be significantly related to physical and biochemical characteristics and clinical diseases [6].

In recent years, there have been various tools for determining nitrogenous bases in the MT-ND5 gene sequence using experimental methods. The chemical, physical, and biological methods make the determination process very complex and time-consuming. The bioinformatics method based on sequence information may lead to significant improvements in the speed and success rate of nitrogenous base determination. The key to the bioinformatics method is to accurately determine the corresponding rule between the content of nitrogenous bases and feature vectors. Currently, there is no appropriate method to address all types of nitrogenous base variations simultaneously [7].

2.1. Types and Significance of Nitrogenous Bases

The gene sequence of MT-ND5 contains four nucleotides: A, T, C, and G. They perform physiological functions of carrying genetic information, transferring genetic information, reading genetic information, and storing genetic information. The biochemical effects of these bases on humans depend on the recognition of these nitrogenous bases in more specific sequences. Because of this particularity, some researchers want to replace or modify the species of these bases in gene sequences so that they can become new gene therapy drugs. This also gives some bases a role outside of providing energy and matter for humans.

2.2. Traditional Methods for Identifying Base Substitutions

The traditional method for examining the nucleotide substitution mutation of the MT-ND5 gene sequence identification is to observe the electropherogram data in computer software. This software usually utilizes fluorescence detection technology to determine DNA fragments and uses a different fluorescence color to describe the bases A, C, G, and T. When evaluating the maximum peak in the chromatogram at each nucleotide position detected to be higher than 50 p.u. and the average peak-to-peak distance, it would be more than 3 p.u. and would appear in different colors [8].

To conduct the base determination, for example, to examine whether an A or a G base is in a heterozygous mutation site, computer software would display two types of base peaks known as heterozygous peaks and also display average peak height ratios. If the value exceeds a specified threshold, the substitution would be considered valid. A significant disadvantage of using the software, however, is the need for microscopic examination to determine the nucleotide substituting residues in these typical mutation cases. The software may produce 'background fluorescence,' which can affect the examination of the results. When the signal is weak, background fluorescence may be generated, and human examination and judgment of the results must be made when they are questioned

3. Viterbi Algorithm

The Viterbi algorithm leverages structural parameters to analyze sequences and uncover hidden relationships. Specifically, it identifies the relationship between the MT-ND5 gene sequence and the three domains using the dynamic programming variable $v_i(t)$. Here, t represents the position within the sequence (including local start and end sites) and is aligned to the observed sequence, traversing through branches of a T-junction-like structure. The algorithm iteratively updates the probability (p) and traceback pointers (tb) step by step as it processes the observed sequence, ultimately determining the most probable path. Each symbol X_i in the gene sequence is mapped to an observable sequence efficiently, without considering the secondary structure of the genes in the three domains. The translation function utilizes combinations such as $X_{ij} + X_k$ to generate i_{ij}-parameters based on two or three branches of the T-junction, respectively. Only the 2D coordinate symbols are affected by the translation function's output [9].

3.1. Limitations and Challenges

Within fast-evolving regions in the mt-genomes, the good organization of the nucleotide sequence on codons is lost. It causes a significant error in the nucleotide substitution counts using information on amino acid replacement. It's possible to consider that the different swarm algorithms have a wider application in molecular bioinformatics. They can be used to solve a wide spectrum of problems that, using different sequences of nucleotides or amino acids, establish based on their distributions between the control sequences, such as motif search, promoter search, gene prediction, analyzing rate of mutations, and so on.

4. Introduction to Swarm Intelligence Algorithms

In the swarm intelligence approach, cutting-edge research proves that groups such as colonies of ants, schools of fish, and colonies of bacteria (in general, collective animal behavior or swarms) are capable of finding good solutions for the problem of optimization. What emerges from simple behavioral rules can be invaluable to our understanding of the process of organizational structure of the collective entities. Recently, swarm intelligence algorithms for problem optimization have gained importance with numerous origins in nature, such as insect swarming, fish schools, plants, microorganisms, and even galaxies. The emergence of the swarm concept arises from collective behavior, where intrinsically decentralized control is derived from simple interaction rules. Three basic elements characterize the swarm: lack of central control, collective behavior evolution, and distributed subprocesses. These features are prevalent in collective entities [10].

OM (Ordinary Individuals Model): The model is composed of N mobile and passive individuals, all within the same environment. These individuals are placed at several distinct points, where their generalized coordinates form an array defined in the search space. In a real swarm, a part of the search space is usually allocated to each agent. The OM model assumptions differ from practical aspects inherent to the classic Individual-based Model with Movement; the first reflects traditional aspects of a mathematical model destined to the analysis of the operation of a hybrid algorithm, while the second deals with a concrete representation of the animal and its movement. Nonetheless, the two models are means for mathematically enhancing local search strategies, random search strategies, visual range effects, and the social structure of artificial and natural swarms. A set of explanatory diagrams about several important search strategies that swarm agents perform when searching in their respective environments has been developed. The search strategies include termite mound searching, caribou mixed search, school behavior, and caribou synchronized motion [11,16,17].

In this study, a two-stage swarm-based optimization algorithm for predicting the position of the substitution for nitrogenous bases and their types in MT-ND5 gene sequences is proposed. Unlike

other previous studies, our study carries out the prediction of nitrogenous base substitutions within a single gene sequence, but multi-class prediction is achieved within a single stage. Whether single-stage or two-stage optimization models are applied, the nitrogenous base substitution models that are handled give good classification performance. Adaptive comparative search, bat algorithm, cat swarm optimization, and a hybrid of smaller optimization algorithms are utilized in the single-stage optimization model, while two-stage optimized methods are constructed with an artificial immune recognition system, whale optimization algorithm, improved differential search algorithm, and a hybrid of smaller optimization algorithms.

4.1. Methodology for Determining Substituted Nitrogenous Bases

In this work, a series of MT-ND5 gene sequences in humans were compared for sequence lengths of up to (1812). An attempt was made to identify nitrogenous base substitutions. When there are large amounts of amino acid substitutions, it is possible to draw new conclusions. However, this is very rare. This additional cost is due to the need to use large amounts of amino acid position data and/or the logistic constraint of the sequence and occurrence of amino acid features by chance. Program matrix for comparing extinct mitochondrial DNA with current human data. Substitutions in MT-ND5 gene sequences are given taking into account the location and genetic code. The search starts with the replacement of new divergent nitrogenous bases corresponding to the calculated differences. The calculations of nitrogenous base substitutions lead to results that are used with a selection rule chosen for biological reasons.

In Swarm Intelligence, the goal is to evolve a population of solutions (candidate state sequences) toward an optimal sequence by minimizing a cost function (which could be related to the log-probabilities of the HMM). Finds the most likely sequence of hidden states given an observed sequence (using HMM parameters such as transition and emission probabilities).

5. Proposed Approach Using Swarm Algorithms

Swarm intelligence algorithms, specifically the Ant colony optimization(ACO), particle swarm optimization(PSO) with time varying acceleration coefficients, and simulated evolution with an integrated learning automaton have been discussed to determine the resultant sequences and substitutions based on the MT-ND5 gene. The proposed approach using these algorithms should be useful for custom splicing, introducing mutations, determining the effects of mutations, and developing gene vectors. Upon comparison between the three algorithms (Viterbi, ACO, PSO), results regarding techniques and applications were studied to determine the agreement of the results method-wise. The devised approach using three swarm intelligence techniques may be employed for multiple nucleotide pairwise analyses of any pair of homologous DNA and/or RNA sequences. Swarm Intelligence Algorithms that we choose PSO and ACO simulated as

Particle Swarm Optimization (PSO): Every particle in PSO represents a potential hidden state sequence. Both the global best (the best sequence discovered by the swarm) and the personal best (the greatest sequence they have discovered thus far) have an impact on the particles' mobility as they scan the search space (possible sequences).

Ant Colony Optimization (ACO): Ants gradually construct solutions (sequences of states) in ACO. Pheromone trails, which are impacted by past successful solutions, and heuristic data, such as the transition and emission probabilities in HMM, determine the likelihood of choosing a particular state at each stage.

Results of the proposed method employing PSO-HMM, ACO-HMM, These techniques are capable of predicting and identifying relevant gene regions and introns [12, 15].

5.1. Cost Function Definition

Establish a cost function that quantifies the degree of "fit" of a potential state sequence. The negative log-likelihood of the observed sequence given a specific hidden state sequence might serve as the cost function for an HMM.

Here's an example of the cost function *f*(state sequence):

$$f(\text{state sequence}) = -\sum_{k=1}^{L} \log\left(a\left(state_{k-1}, state_k\right)\right) + \log\left(e\left(state_k, observation_k\right)\right) \tag{1}$$

Where:

- a is the transition probability matrix.
- e is the emission probability matrix.
- $state_k$ is the hidden state at position k.
- $observation_k$ is the observed sequence at position k.

The cost function f(state sequence) for decoding a Hidden Markov Model (HMM) indicates the "fitness" of a candidate state sequence based on the HMM's transition and emission probabilities. In layman's terms, it assesses how well a given series of hidden states (such as 'A', 'T', 'C', and 'G') describes the observed sequence.

1- Transition Costs:

$$\log(a(state_{k-1}, state_k)) \tag{2}$$

these account for the probabilities of moving from one state to the next. For each transition from $state_k$ to $state_k$, you compute the *log* of the corresponding transition probability a($state_{k-1}$,$state_k$).

2- Emission Costs:

$$\log(e(state_k, obs_k)) \tag{3}$$

these account for how likely the observed symbols are, given the hidden states. For each state $state_k$, you compute the log of the emission probability $e(state_k, obs_k)$ (the likelihood of observing obs_k in state $state_k$.

3- Total Cost:

The sum of all negated transition and emission costs is the total cost function (1). Because a lower cost translates into a higher likelihood, minimizing this cost is equivalent to identifying the most likely state sequence.

In this section, substitution mutations were applied to the MT-ND5 gene sequence of humans to compare the matching ratio of the two sequences that can be obtained from the substitution process. The intelligent swarm algorithm was used instead of the traditional algorithm used to determine the type of the nitrogenous base substituted for the MT-ND5 gene. The following algorithm was proposed to determine the type of the nitrogenous base substituted for the MT-ND5 gene for both humans and mice as follows:

Proposed intelligent algorithm for determining the type of substituted nitrogenous base:

Process 1: The four nitrogenous bases are encoded by converting the letter symbols into numbers which form the DNA chain as follows

$$A = 1,\ T = 2,\ C = 3,\ G = 4$$

Process 2: Definition of the elements of the hidden Markov model λ = (A, B, π), where π represents the vector of the initial state with dimensions 1**N*, and *N* = 4 represents the number of states. As for *A*, it represents the matrix of transitional probabilities between the hidden states, whose dimensions

are generally ($N*N$). And B represents the probability matrix linking the hidden states and the observations (the matrix of versions) with dimensions ($N*M$), where $M = 3$.

Process 3: Try substituting one of the rules (A, T, C, G) with(A, T, C, G) and counting all of the choices, which total 12.

Process 4: Finding potential hidden states using an intelligent algorithm, ACO or PSO. We can say solve the dynamical programming problem (1) using ACO or PSO.

Process 5: The series of cases resulting from step 4 is compared with the series of real cases. In this step, the type of the replaced nitrogenous base is estimated with its corresponding series of cases resulting from step 4. The Mean Squares Error (MSQ) and Match Ratio (MR) are found according to the mathematical equations (… and …).

$$MSQ = \frac{1}{L}\sum_{i}(q - Decode)^2$$

Where, Q represents the true hidden states,
$decode$ represents the encrypted hidden states,
and L indicates the chain's length.

$$MR\% = ((L - sum(error)) \mid L) * 100$$

($error$): denotes the logical expression vector and the error vector with dimension ($L \times 1$).

6. Experimental Setup and Data Collection

6.1. Data Preprocessing and Feature Selection

Before executing a swarm intelligence algorithm, the original dataset should be normalized into values {1,2,3}. The primary sequence of the DNA consists of the A, T, C, or G bases. The biological system was defined with four types of genetic elements representing the individual structural components. The components define the human mitochondrial genome, e.g., the MT-ND5 gene.

6.2. Parameters and Settings for Swarm Algorithms

Parameter	PSO (Particle Swarm Optimization)	ACO (Ant Colony Optimization)
Number of Particles/Ants	num_particles (e.g., 30)	num_ants (e.g., 30)
Number of Iterations	max_iter (e.g., 100)	num_iterations (e.g., 100)
Inertia Weight (w)	w (e.g., 0.5)	Not applicable
Cognitive Parameter (c1)	c1 (e.g., 1.5)	Not applicable
Social Parameter (c2)	c2 (e.g., 1.5)	Not applicable
Velocity Initialization	Random initialization (zeros by default)	Not applicable
Pheromone Matrix (τ)	Not applicable	pheromone (initialized with small positive values)
Heuristic Information (η)	Not applicable	heuristic (inverse of probabilities, optional)
Pheromone Decay Rate (ρ)	Not applicable	rho (e.g., 0.5)
Pheromone Deposit Amount (Q)	Not applicable	Q (e.g., 1.0, affects pheromone addition)
Alpha (α)	Not applicable	alpha (e.g., 1.0, weight of pheromone importance)

Beta (β)	Not applicable	beta (e.g., 2.0, weight of heuristic importance)
Solution Construction	Update position based on velocity	Construct solutions using probability-based state selection
Personal Best (pBest)	Tracked for each particle	Not applicable
Global Best (gBest)	Tracked for the entire swarm	Tracked as the best solution found
Fitness/Cost Function	Custom function to evaluate each particle	Custom function to evaluate each ant's solution

6.3. Results and Analysis

Convert			A→C	A→T	A→G	C→A	C→T	C→G	G→A	G→C	G→T	T→A	T→C	T→G
ACO-HHM		MR	68.0464	72.8477	81.2362	66.8874	72.4614	78.9183	81.6777	79.0287	84.6026	72.6821	71.468	83.6093
		MSE	1.2781	0.27152	1.6887	1.3245	0.27539	0.21082	1.649	0.20971	0.61589	0.27318	0.28532	0.65563
PSO-HHM		MR	25.2208	24.7792	26.1038	24.9448	25.4967	24.3929	25.883	24.3377	25.5519	24.8344	24.3377	25.4415
		MSE	2.3173	2.3874	2.3206	2.3096	2.3184	2.3306	2.3582	2.3411	2.3422	2.3725	2.2914	2.3482

6.4. Discussion and Implications

In conclusion, a comparison of the results and computations yields a simple procedure for solving a complex problem of dynamical programming of Viterbi methods. In summary, the application of the group swarm algorithms should be useful for conducting an evolutionary spectroscopy selection of the most significant group of spectral features from a very large set of possibilities. Such a selection can be significant in a variety of applied fields, particularly in quantitative spectral analysis, DNA sequencing, and function prediction, such as analyzing gene sequences for overlapping coding regions and hidden stop codons.

6.5. Interpretation of Results

After studying the design of swarm algorithms for solving mathematical programming, which was derived from the study of the maximum likelihood of obtaining the truth chain after applying the hidden Markov chain, we need to conduct an application to verify its effectiveness. We derived the design by studying the human gene sequence MT-ND5. We achieved very low square errors (0.2), and we also reached 84% matching rates. Some bases were not found. We obtain a set of possible functional formulas for the quasi-specific types of the ND5 gene sequences. With four bases at a

certain distance, the goal was to obtain a set of quasi-specific types for all possible distances from the human gene sequence to each functional formula. This will aid in understanding the interaction windows within the ND5 gene. Additionally, it enables the identification of quasi-specific gaps in the sequences. For cases of four bases per sequence, it was possible to obtain quasi-specific types for some functional formulas.

This paper has the potential to develop into a series of papers on sequence data analysis using hybrid manipulations of the swarm algorithm. Future publications will delve into the entire mitochondrial DNA molecule, conducting more base data substitution experiments and examining the hydration rules associated with the substituents. Another area of interest is the algorithm's ability to assign appropriate base substitutions for comparing homologous and analogous protein subunits. We can apply swarm intelligence algorithms as optimization techniques to HMM decoding. While ACO is more straightforward than PSO in its application to sequence optimization, it can be more flexible when dealing with situations such as HMM decoding, where sequence selections at each step are influenced by both local and global information.

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