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Finite element inverse analysis using a photosynthetic algorithm

Haruhiko Murase

Department of Regional Environmental Science, Laboratory of Phytotronics and Sensibility Engineering, Osaka Prefecture University, 1-1, Gakuen, Sakai 599-8531, Japan

Abstract

The reaction of carbon molecules in the dark reaction of photosynthesis was chosen as a biosystem-derived algorithm (BDA). This study refers to the BDA as the photosynthetic algorithm (PA). The PA utilizes the rules governing the transfer of carbon molecules from one substance into another in the Benson–Calvin cycle and photorespiration reactions. The mechanism of PA is an organized random search biomimetically rationalized by photosynthetic processes. This paper presents the principles of the PA in detail. A finite element inverse analysis was selected as a typical optimization or parameter estimation problem to demonstrate the performance of the PA. The elastic moduli of a finite element model were successfully estimated from predetermined boundary conditions and observed deformation data. © 2000 Elsevier Science B.V. All rights reserved.

Keywords: Photosynthetic algorithms; Biosystem derived algorithm; Dark reaction; Benson-Calvin cycle; Photorespiration; Local minimum trap; Optimization methods

1. Introduction

A number of problems in the discipline of agricultural engineering involve the optimization of different types of operating systems, such as drainage and irrigation systems, crop scheduling, and the handling and blending of materials. Such operating systems typically depend upon decision parameters that can be chosen by the system designer or operator. An inappropriate choice of decision parameters causes serious flaws in the performance of such a system, as measured by some relevant objective or fitness function. Another problem often encountered in the discipline of agricultural engineering lies in the field of testing and fitting

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quantitative models. Engineering or scientific research in any problem area classically consists of an iterative process of building explanatory or descriptive models. collecting data, testing the models, modifying the models when discrepancies are found, and then repeating the process until the problem is solved. The problems that deal with optimizing operating systems and fitting quantitative models eventually require some treatment or processing using adaptive search procedures or optimization techniques. There are many search techniques, such as exhaustive techniques (random walk), calculus-based techniques (gradient methods), partial knowledge techniques (hill climbing), knowledge-based techniques (production rule systems, heuristic methods), stochastic techniques (simulated annealing), and biosystem-originated algorithms (genetic algorithm, immune system algorithm). In realistic systems, the interactions between the parameters are not generally amenable to analytical treatment, and the researcher must resort to appropriate search techniques. Recently, genetic algorithms and immune system algorithms have received attention, due to their ability to locate very good approximate solutions in extremely large search spaces with a reasonable computational load (Farmer et al., 1986; Goldberg, 1989).

It is interesting to note that if one looks carefully at plant systems or phytosystems, many different biosystem-derived algorithms (BDA) can be found. Photosynthesis is one of the most important biochemical phenomena. The most interesting photosynthetic reactions are the set known as the 'dark reactions'. The dark reactions are the biochemical processes that combine the Benson-Calvin cycle and reactions of photosynthesis consist of the set known as the 'dark reactions'. The dark reactions comprise a biochemical process consisting of a combination of the Benson-Calvin cycle and photorespiration. The product of the dark reactions is carbohydrate. The biochemical balance between the Benson-Calvin cycle and photorespiration can be viewed as a natural implementation of an optimization procedure that maximizes the efficiency of sugar production under the continuous variation of energy input from the sun. It is sometimes maintained that a plant is not optimized by nature to function as an energy conversion device, because of its very low energy conversion efficiency of about three percent. Comparisons are made to man-made devices such as photovoltaic cells and photoelectrochemical cells, which transform the sun's energy into an electrical current, or chemical fuels with an efficiency as high as 25%. This is not a fair comparison, however, because plants are under heavy functional constraints to maintain the diverse set of biological activities necessary for their survival and for the preservation of their species. A fair comparison would require that only those biochemical pathways in the plant directly related to energy conversion be considered when calculating energy conversion efficiency.

The author has developed a new BDA using the mechanism of the photosynthetic pathway. In the present study the process of the reaction of carbon molecules in the dark reaction of photosynthesis is chosen as a BDA. The BDA is referred to as the 'photosynthetic algorithm (PA)'. In the next section, the principles of the PA are presented. Subsequently, the application of the PA to typical estimation problems is discussed.

2. Principle of PA

Fig. 1 shows a diagram of the Benson-Calvin cycle (Bowyer and Leegood, 1997). In this diagram, each line represents the conversion of one molecule of each metabolite. The cycle can be divided into three phases.

The first phase of the Benson–Calvin cycle is a carboxylation, catalyzed by ribulose bisphosphate carboxylase (Rubisco). The second phase is the reductive phase in which glycerate-3-P (3PG) is reduced to triose-P by the actions of glycerate-3-P kinase and NADP-dependent glyceraldehyde-P dehydrogenase. The third phase involves the regeneration of the acceptor, ribulose-1,5-P of the sugar phosphate shuffle, in which five C_3 units are converted into three C_5 units.

Rubisco is a bifunctional enzyme which catalyzes both the carboxylation and the oxygenation of RuBP. Oxygenation of RuBP leads to the production of one

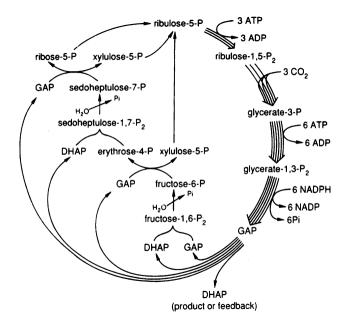


Fig. 1. Benson-Calvin cycle.

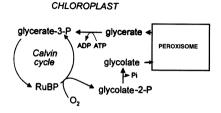


Fig. 2. Photorespiration.

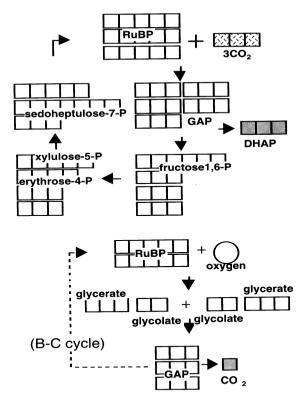


Fig. 3. Recombination of carbon molecules in the B-C cycle (above) and photorespration (below).

molecule of 3PG and one of glycolate-2-P. Fig. 2 shows the part of the photorespiratory pathway that is dependent upon Rubisco.

The PA utilizes the rules governing the conversion of carbon molecules from one substance to another in the Benson-Calvin cycle and photorespiration reactions. Fig. 3 illustrates the variation of recombination of carbon molecules appearing in the PA. The first phase of the Benson-Calvin cycle and the reaction taking place in the chloroplast subcellular compartment for photorespiration were utilized for the algorithm. The product of photosynthesis, DHAP as shown in Fig. 1, serves to provide the knowledge strings of the algorithm. Optimization is attained when the quality of the products no longer improves. The quality of a product is evaluated based on the fitness value. The fitness value can be obtained by calculating the difference between the output value of the system using parameters currently given by the PA and the training output data. Fig. 4 shows a flow diagram indicating the calculation process of the PA. The process start with the random generation of light intensity. CO₂ fixation rate is then evaluated by Eq. (1) based on the light intensity. Depending on the fixation rate, either Benson-Calvin cycle or photorespiration cycle is chosen for the next process. In the both cycles, Sixteen bits strings are shuffled according to carbon molecules recombination rule in photosynthetic pathways. After some iterations, GAPs which are intermediate knowledge strings are produced. Each GAP consists of 16 bits. The fitness of these GAPs are then evaluated. The best fit GAP remains as a DHAP (current estimated value). One of the unique features of the algorithm is that the stimulation function is provided. The stimulation occurs due to randomly changing light intensity which alters the degree of influence on renewing the elements of RuBP by photorespiration. The frequency of the stimulation cycle by photorespiration can be calculated by the CO₂ fixation rate given by Eq. (1).

$$C = V_{\text{max}}/(1 + A/L) \tag{1}$$

where C is the CO_2 fixation rate; V_{max} is the maximum CO_2 fixation rate; A is the affinity of CO_2 ; and L is the light intensity.

The parameters involved in Eq. (1) are all determinable, but these values can be assigned within a realistic range and need not be empirical. When executing the PA, the light intensity (L) should be generated randomly by computer. Alternatively, the actual light intensity varying with time through an on-line measuring system might be used. The variation of the light intensity as a stimulation is effective in reducing the occurrence of local minimum traps in the search process. The $\rm CO_2$ concentration in the leaf varies depending on the $\rm CO_2$ fixation rate. The ratio of $\rm O_2$ concentration and $\rm CO_2$ concentration is evaluated to determine the ratio of the calculation frequency of the Benson–Calvin cycle to that of the photorespiration cycle.

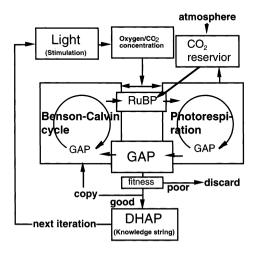


Fig. 4. The photosynthetic algorithm.

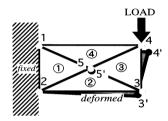


Fig. 5. Finite element model (Cantilever beam).

3. Finite element inverse analysis by PA

A finite element inverse analysis is an example of a typical optimization or parameter estimation problem. There are calculus-based estimation techniques, such as the least square, conjugate gradient, and Kalman filter methods (Murase et al., 1994), available for solving finite element inverse problems. BDA may also be used for finite element inverse problems, even though few studies have been reported. In this section, the performance of the PA in solving a finite element inverse problem is discussed. A cantilever beam system (5 unit length × 10 unit length) is provided for a numerical example as illustrated in Fig. 5. The finite element model consisting four linear triangular elements is used as an example finite element structure. The elastic properties (Young's modulus and Poisson's ratio) of each element are assumed to differ. Nodes 1 and 2 are fixed. The remaining nodes can be displaced freely. A unit vertical load is applied at node 4. The displacements of nodes 3, 4 and 5 in the horizontal and vertical directions due to the unit load are observed. The PA is expected to search for the optimum values of the eight unknown elastic moduli, which are the Young's modulus and Poisson's ratio of each finite element.

The parameters used for this test were as follows: the affinity of CO_2 was set to 10 000; the maximum light intensity varied from 10 000 to 50 000 lux (an increase in light intensity implies an increase in the chance to activate photorespiration); the maximum CO_2 fixation speed was 30; and the maximum number of cycles for the Benson–Calvin cycle and photorespiration were 30 and 45, respectively, per search iteration.

Fig. 6 illustrates the procedure for the finite element inverse analysis using the PA. As shown in Fig. 6, the finite element evaluation appears in the process of the fitness check of the knowledge strings (DHAP) indicated at the end of the flow diagram. Each of the eight elastic moduli is coded in a 16-bit DHAP molecule. After converting them into decimal numbers, the nodal displacements at nodes 3, 4 and 5 are calculated using the estimated elastic moduli and the given boundary conditions. The observed displacement data are compared with the calculated output data to obtain the fitness of the estimates. When a set of estimates with better fitness than the previous data are obtained, the best data set is stored in the DHAP reservoir for the next comparison. After completing one cycle of the search process with a predetermined frequency for the Benson–Calvin cycle and

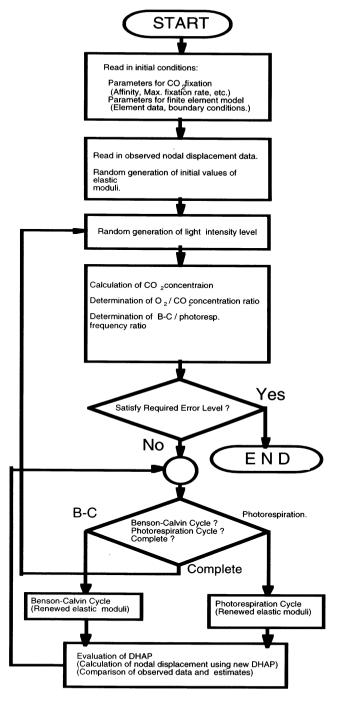


Fig. 6. Flow diagram of finite element inverse analysis by PA.

photorespiration, the process then randomly generates the light intensity for the next iteration with a renewed photosynthetic frequency condition.

The observed displacements at nodes 3, 4, and 5 are indicated in Table 1. The negative values of Y imply that nodes 3, 4 and 5 are displaced downward by the force applied at node 4. In this simulation, the observed displacements were calculated from the predetermined elastic moduli. These predetermined elastic values are supposed to be the target values in the estimation test.

4. Results and discussion

The estimation of the elastic moduli of the finite element model using the PA was very satisfactory. Fig. 7 shows the convergence property of the fitness. A dramatic decline in the error level down to 10^{-4} was observed in the initial ten0 iterations. After 1000 iterations, the PA converged at the total absolute error level of $\sim 2.8 \times 10^{-4}$. No significant improvement was observed after 200 iterations. Tables 2 and 3 summarize the comparison of the estimated values of the elastic moduli (Young's modulus and Poisson's ratio) and corresponding target values. The tables show that most of the estimated values are very close to their target values except the Poisson's ratio of element number 4.

Table 1 Observed displacements at nodes 3, 4 and 5

Node	Displacement		
	\overline{X}	Y	
3	-0.0332	-0.123	
4	0.4140	-1.303	
5	0.0011	-0.055	

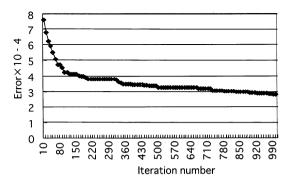


Fig. 7. Convergence property of estimates.

Table 2
Estimated values of Young's modulus

Element	Estimated	Target
1	116	120
2	80	80
3	95	90
4	68	70

Table 3
Estimated values of Poisson's ratio

Element	Estimated	Target
1	0.24	0.25
2	0.30	0.35
3	0.29	0.30
4	0.23	0.32

5. Conclusion

This study demonstrated the effectiveness of the PA in estimation. The PA is a newly-developed algorithm that can be used for search and optimization problems. It is important to note that the PA is derived from a biosystem. Biosystems consist of many different natural phenomena, many of which are very peculiar and impressive. The genetic immune system, and PAs are all BDA. There are surely many other algorithms represented in biosystems that might prove useful in engineering applications. Seeking useful engineering principles exemplified in biosystems is likely to be a fruitful path to advances in bioengineering.

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