NEURAL NETWORK SIMULATION OF SIMPLE BIOLOGICAL SYSTEMS INCLUDING OPTIMAL CONTROL PROBLEMS

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ABSTRACT
The mechanistic model of the phytoplankton photosynthesis-light intensity relationship and nitrogen transformation cycle are investigated. Assuming that phytoplankton regulates its photosynthetic production rate with certain strategy which maximizes photosynthetic and biomass production, respectively two such possible strategies were examined using a neural network based optimal control synthesis for solving fixed and free final time optimal control problems with control and state constraints. The optimal control problem is transcribed into nonlinear programming problem which is implemented with adaptive critic neural network. Results show that adaptive critic based systematic approach holds promise for obtaining the fixed and free final time optimal control with control and state constraints.

Keywords: optimal control problem, state and control constraints, free terminal time, neural network simulation, phytoplankton photosynthesis, nitrogen transformation cycle, optimal photosynthetic production

1. INTRODUCTION
Optimal control of nonlinear systems is one of the most active subjects in control theory. There is rarely an analytical solution although several numerical computation approaches have been proposed (for example, see (Kirk, 1989), (Polak, 1997). The most of the literature dealing with numerical methods for the solution of general optimal control problems focuses on algorithms for solving discretized problems. The basic idea of these methods is to apply nonlinear programming techniques to the resulting finite dimensional optimization problem (Buskens, Maurer, 2000). When Euler integration methods are used, the recursive structure of the resulting discrete time dynamic can be exploited in computing first-order necessary condition.

In the recent years the neural networks are used for obtaining numerical solutions to optimal control problem (Padhi, Unnikrishnan, Wang, and Balakrishnan, 2001), (Padhi, Balakrishnan and Randoltph, 2006). For the network, a feed forward network with one hidden layer, a steepest descent error backpropagation rule, a hyperbolic tangent sigmoid transfer function and a linear transfer function were used.

The paper presented extends adaptive critic neural network architecture proposed by Padhi, Unnikrishnan, Wang and Balakrishnan (2001) to the optimal control problems with control and state constraints. The organization of the paper is as follows. In Section 2 optimal control problems with control and state constraints are being introduced. We summarize necessary optimality conditions and give a short overview on basic result including iterative numerical methods and discussed discretization methods for given optimal control problem and a form of resulting nonlinear programming problems. Section 3 presented a short description of adaptive critic neural network synthesis for optimal problem with state and control constraints. Section 4 consists of a mechanistic model of phytoplankton photosynthesis. We prove the existence of unique globally asymptotically stable equilibrium depending on light intensity. Using optimal control theory we maximize photosynthetic production rate for fixed and free final time. Section 5 presented a nitrogen transformation cycle. We investigate a preferential utilization of nitrogen compounds by phytoplankton using adaptive critic neural network. We examine short and long-term strategy of utilization. Conclusions are being presented in Section 6.

2. OPTIMAL CONTROL PROBLEM
We consider nonlinear control problem subject to control and state constraints. Let $x(t) \in R^n$ denote the state of a system and $u(t) \in R^m$ the control in a given time interval $[t_0, t_f]$.
Optimal control problem is to minimize

$$J(x,u) = g\left(x(t_f)\right) + \int_{t_0}^{t_f} f_0\big(x(t),u(t)\big)dt \qquad (1)$$

subject to

$$\dot{x}(t) = f\big(x(t),u(t)\big),$$

$$x(t_0) = x_0,$$

$$\psi(x(t_f)) = 0,$$

$c(x(t),u(t)) \le 0,\ \ t \in [t_0,t_f].$

The functions $g: R^n \to R$, $f_0: R^{n+m} \to R$, $f: R^{n+m} \to R^n, c: R^{n+m} \to R^q$ and $\psi: R^{n+m} \to R^r, 0 \le r \le n$ are assumed to be sufficiently smooth on appropriate open sets. The theory of necessary conditions for optimal control problem of form (1) is well developed (Kirk, 1989), (Pontryagin, Boltyanskii, Gamkrelidze and Mischenko, 1983).

We introduce an additional state variable

$$x_0(t) = \int_0^t f_0(x(s),u(s))ds$$

defined by the

$\dot{x}(t) = f_0(x(t),u(t)), x_0(0) = 0.$

Then the augmented Hamiltonian function for problem (1) is

$$H(x,\lambda,\mu,u) = \sum_{j=0}^{n} \lambda_j f_j(x,u) + \sum_{j=0}^{q} \mu_j c_j(x,u), \qquad (2)$$

where $\lambda \in R^{n+1}$ is the adjoint variable and $\mu \in R^q$ is a multiplier associated to the inequality constraints. Let $(\hat{x},\hat{u})$ be an optimal solution for (1) then the necessary condition for (1) (Kirk, 1989), (Pontryagin, Boltyanskij, Gamkrelidze and Mischenko,1983) implies that there exist a piecewise continuous and piecewise continuously differentiable *adjoint function* $\lambda: [t_0,t_f] \to R^q$, $\mu(t) \ge 0$ and a multiplier $\sigma \in R^r$ satisfying

$$\dot{\lambda}_j(t) = -\frac{\partial H}{\partial x_j}(\hat{x}(t),\lambda(t),\mu(t),\hat{u}(t))$$

$$\lambda_j(t_f) = g_{x_j}\left(\hat{x}(t_f)\right) + \sigma\psi_{x_j}\left(\hat{x}(t_f)\right), j = 0,\dots,n \quad (3)$$

$$\dot{\lambda}_0(t) = 0$$

$$0 = \frac{\partial H}{\partial u}(\hat{x}(t),\lambda(t),\mu(t),\hat{u}(t)).$$

For free terminal time t_f, an additional condition needs to be satisfied:

$$H(t_f) = (\sum_{j=0}^{n} \lambda_j f_j(x,u) + \sum_{j=0}^{q} \mu_j c_j(x,u))|_{t_f} = 0.$$

Furthermore, the complementary conditions hold i.e. in $t \in [t_0,t_f]$, $\mu \ge 0$, $c(x,u) \le 0$ and $\mu\, c(x,u) = 0$. Herein, the subscript x or u denotes the partial derivative with respect to x or u.

2.1. Discretization of optimal control problem

Direct optimization methods for solving the optimal control problem are based on a suitable discretization of (1). Choose a natural number N and let $t_i \in [t_0,t_f], i = 1,\dots,N-1$, be an equidistant mesh point with $t_i = t_0 + ih$, $i = 1,\dots,N$, where h is time step and $t_f = Nh + t_0$. Let the vectors $x^i \in R^{n+1}, u^i \in R^m$, $i = 1,\dots,N$, be approximation of state variable and control variable $x(t_i)$, $u(t_i)$, respectively at the mesh point. *Euler's* approximation applied to the differential equations yields

$$x^{i+1} = x^i + hf(x^i,u^i), \qquad i = 0,\dots,N-1.$$

Choosing the optimal variable $z := (x^0,x^1,\dots,x^{N-1},u^0,\dots,u^{N-1}) \in R^{N_s}, N_s = (n+1+m)N$, the optimal control problem is replaced by the following discretized control problem in the form of nonlinear programming problem with inequality constraints:

$min\, J(z) = G(x^N),$

where

$$G(x^N) = g((x_1,\dots,x_n)^N, t_N) + x_0^N, \qquad (4)$$

subject to

$$-x^{i+1} + x^i + hf(x^i,u^i) = 0,$$

$$x^0 = x(t_0),$$

$$\psi(x^N) = 0,$$

$$c(x^i,u^i) \le 0,\ \ i = 0,\dots,N-1.$$

In a discrete-time formulation we want to find an admissible control which minimizes object function (4). Let us introduce the Lagrangian function for the nonlinear optimization problem (4):

$$L(z,\lambda,\sigma,\mu,h) = \sum_{i=0}^{N-1} \lambda^{i+1}(-x^{i+1} + x^i + f(x^i,u^i)) +$$
$$+G(x^N,t_N) + \sum_{i=0}^{N-1} \mu^i c(x^i,u^i) + \sigma\psi(x^N,t_N). \qquad (5)$$

and define $H(i)$ and Φ as a follows:

$H(i) = \lambda(i+1)(x^i + hf(x^i,u^i),$
$\Phi = G + \sigma\psi.$

The first order optimality conditions of Karush-Kuhn-Tucker (Polak, 1997) for the problem (4) are:

$$0 = L_{x^i}(s,\lambda,\mu,h) = \lambda^{i+1} + h\lambda^{i+1} f_{x^i}(x^i,u^i) - \lambda^i + \mu^i c_{x^i}(x^i,u^i), i = 0,\dots,N-1, \quad (6)$$

$$0 = L_{x^N}(s, \lambda, \mu, h) \\ = G_{x^N}(x^N) + \sigma\psi_{x^N}(x^N, t_N) - \lambda^N \quad (7)$$

$$0 = L_{u^i}(s, \lambda, \mu, h) = h\lambda^{i+1} f_{u^i}(x^i, u^i) + \mu^i c_{u^i}(x^i, u^i), \\ i = 0, \dots, N-1, \quad (8)$$

$$0 = L_h(s, \lambda, \mu, h) = \Phi_h + \sum_{i=0}^{N-1} H_h(i) \\ + \sum_{i=0}^{N-1} \mu^i c_h(x^i, u^i), \quad (9)$$

Eq. (6-9) represents the discrete version of necessary condition (3) for optimal control problem (1).

3. ADAPTIVE CRITIC NEURAL NETWORK FOR OPTIMAL CONTROL PROBLEM WITH CONTROL AND STATE CONSTRAINTS AND FREE TERMINAL CONDITION

It is well known that a neural network can be used to approximate smooth time-invariant functions and uniformly time-varying function (Hornik, Stichcombe and White, 1989), (Sandberg, 1998). Neurons are grouped into distinct layers and interconnected according to a given architecture (Figure 1). Each connection between two neurons has a weight coefficient attached to it. The standard network structure for an approximation function is the multiple-layer perceptron (or feed forward network). The feed forward network often has one or more hidden layers of sigmoid neurons followed by an output layer of linear neurons.

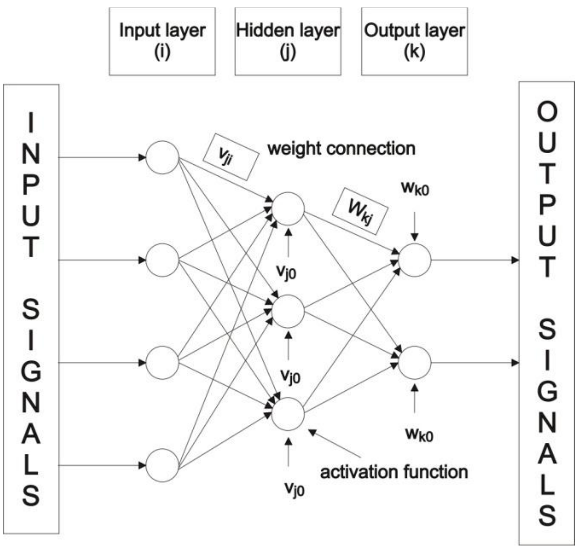

Figure 1: Feed Forward Neural Network Topology with One Hidden Layer (v_{ji}; w_{kj} are values of connection weights, v_{j0}; w_{k0} are values of bias)

Figure 1 shows a feed forward neural network with n_i inputs nodes one layer of n_{hl} hidden units and n_o output units. Let $in = [in_1, \dots, in_{n_i}]$ and $out = [out_1, \dots, out_{n_o}]$ be the input and output vectors of the network, respectively. Let $V = [v_1, \dots, v_{n_{hl}}]$ be the matrix of synaptic weights between the input nodes and the hidden units, where $v_j = [v_{j0}, v_{j1}, \dots, v_{jn_i}]$ and v_{j0} is the bias of the *j*th hidden unit.

Let also $W = [w_1, \dots, w_{n_o}]$ be the matrix of synaptic weights between the hidden and output units, where $w_k = [w_{k0}, w_{k1}, \dots, w_{kn_o}]$ and w_{k0} is the bias of the *k*th output unit, w_{kj} is the weight that connects the *j*th hidden units to the *k*th output unit.
The response of the *j*th hidden unit is given by

$$hl_j = tanh(\sum_{i=0}^{n_i} v_{ji} in_k),$$

where $tanh(.)$ is the activation function for the hidden units. The response of the *k*th output unit is given by

$$out_k = \sum_{j=0}^{n_{hl}} w_{kj} hl_j.$$

Multiple layers of neurons with nonlinear transfer functions allow the network to learn nonlinear and linear relationships between input and output vectors. The number of neurons in the input and output layers is given, respectively, by the number of input and output variables in the process under investigation.

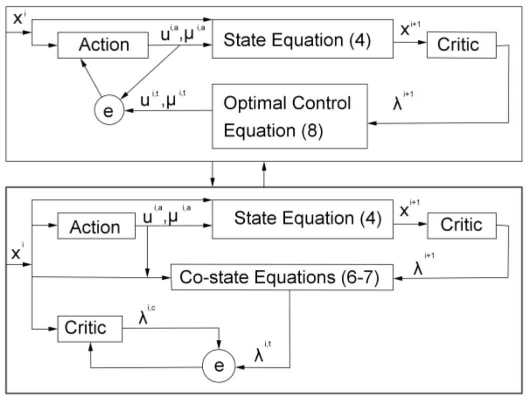

Figure 2: Architecture of Adaptive Critic Network Synthesis

The multi-layered feed forward network shown in Figure 2 is training using the steepest descent error backpropagation rule. Basically, it is a gradient descent, parallel distributed optimization technique to minimise the error between the network and the target output (Rumelhart, Hinton and Wiliams, 1987).

In the Pontryagin's maximum principle for deriving an optimal control law, the interdependence of the state, costate and control dynamics is made clear. Indeed, the optimal control $\hat{u}$ and multiplier $\hat{\mu}$ is given by Eq. (8), while the costate Eqs. (6-7) evolves backward in time and depends on the state and control. The adaptive critic neural network is based on this relationship. It consists of two networks at each node: an action network the inputs of which are the current states and outputs are the corresponding control $\hat{u}$ and multiplier $\hat{\mu}$, and the critic network for which the current states are inputs and current costates are outputs for normalizing the inputs and targets (zero mean and standard deviations). For detail explanation see (Rumelhart, Hinton and Wiliams, 1987), (Kmet, 2011).

From free terminal condition ($\psi(x) \equiv 0$) and from Eqs. (6-7) we obtain that $\lambda_0^i = -1$ for $i = N,\dots,0$ and $\lambda_j^N = 0$ for $j = 1,\dots, n$. We use this observation before proceeding to the actual training of the adaptive critic neural network. The steps for training the action network are as follows:

1) Generate set S. For all $x^k \in S$, follow the steps below:
(1.i) Input x^k to the action network to obtain $u^{k;a}$ and $\mu^{k;a}$.
(1.ii) Using x^k and $u^{k;a}$ solve state equation (4) to get x^{k+1}.
(1.iii) Input x^{k+1} to the critic network to obtain μ^{k+1}.
(1.iv) Using x^k and μ^{k+1} solve (8) to calculate $u^{k;t}$ and $\mu^{k;t}$.

When

$$\|(u^{k,a},\mu^{k,a}) - (u^{k,t},\mu^{k,t})\| \,/\, \|(u^{k,t},\mu^{k,t})\| < \epsilon_a,$$

the convergence criterion for the action network training is met.

The training procedure for the critic network which expresses the relation between x^k and λ^k is as follows:

1) Generate set S. For all $x^k \in S$, follow the steps below:
(1.i) Input x^k to the action network to obtain $u^{k;a}$ and $\mu^{k;a}$.
(1.ii) Using x^k and $u^{k;a}$ solve state equation (4) to get x^{k+1}.
(1.iii) Input x^{k+1} to the critic network to obtain λ^{k+1}.
(1.iv) Using x^k , $u^{k,a}$, $\mu^{k,a}$ and λ^{k+1} solve (6) to calculate $\lambda^{k,t}$.
(1.v) Input x^k to the critic network to obtain $\lambda^{k,c}$.

When

$$\|\lambda^{k,c} - \lambda^{k,t}\| \,/\, \|\lambda^{k,t}\| < \epsilon_c,$$

the convergence criterion for the action network training is met.

Further discussion and detail explanation of this adaptive critic method can be found in (Hornik, Stichcombe, White, 1989), (Padhi, Unnikrishnan, Wang and Balakrishnan, 2001), (Padhi, Balakrishnan and Randoltph, 2006), (Werbos, 1992),.

4. A MECHANISTIC MODEL OF PHYTOPLANKTON PHOTOSYNTHESIS

Mathematical models of photosynthesis in bioreactors are important for both basic science and the bioprocess industry (Garcia-Camacho et al., 2012). There is a class of models based on the concept of the "photosynthetic factories" developed by Eilers and Peeters (1988). The dynamic behaviour of the model has also been discussed in (Eilers and Peeters, 1993), (Kmet, Straskraba and Mauersberger 1996), (Papacek, Celikovsky, Rehak and Stys, 2010), (Wu and Merchuk, 2001) Assuming that phytoplankton regulates its photosynthetic production rate with a certain strategy which maximize production, two such possible strategies is examined, i.e. instantaneous and the integral maximal production.

4.1. Description of the Model

Basic for the following consideration is the mechanistic model of phytoplankton photosynthesis. It is based on unit processes concerning the cellular reaction centres called photo-synthetic-factories - PSF. It is known from algal physiology (Eilers, Peeters, 1988) that three states of a PSF are possible: x_1- resting, x_2 - activated and x_3 - inhibited. Transitions between states depend both on light intensity and time. The probabilities of the PSF being in the state x_1, x_2 or x_3, are given as p_1, p_2 and p_3, respectively. Transitions between states can be expressed as follows:

$$\begin{aligned} \dot{p}_1 &= -\alpha I p_1 + \gamma p_2 + \delta p_3 \\ \dot{p}_2 &= \alpha I p_1 - (\beta I + \gamma) p_2 \\ \dot{p}_3 &= \beta I p_2 - \delta p_3. \end{aligned} \tag{10}$$

The parameters α, β, γ and δ occurring in this model are positive constants and I is a light intensity.

Let $p(t, p^0)$ be a solution of (10) with the initial condition $p(0, p^0) = p^0$, where $p_1^0 + p_2^0 + p_3^0 = 1$. Note that solutions of the system (10) exist for all $t \geq 0$. By adding up the right-hand side of (10) we get

$$\dot{p}_1 + \dot{p}_2 + \dot{p}_3 = 0,$$

i.e. $\sum_{i=1}^{3} p_i(t, p^0) = 1$ for all $t \geq 0$. Of course these equations are considered in

$$S = \{p \in R_+^3 : p_1 + p_2 + p_3 = 1\}.$$

4.2. Global behaviour under constant condition

Proposition. *Let parameters $\alpha, \beta, \gamma, \delta$ and I be positive, then there exists an unique positive equilibrium $\bar{p}$ which is globally asymptotically stable on S.*

Proof: Vector $\bar{p}$ is the solution of the following linear equation system:

$$P \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \tag{11}$$

where

$$P = \begin{pmatrix} -\alpha I & \gamma & \delta \\ \alpha I & -\beta I - \gamma & 0 \\ 0 & \beta I & -\delta \end{pmatrix}.$$

Let us consider the matrix $D = P + \rho E$, where $\rho = max|P_{ii}|$ and E is the unit matrix. D is an irreducible nonnegative matrix and so the apparatus of the Perron-Frobenius theory of a nonnegative matrix applies. Since $1P = 0$, also $1D = \rho 1$, where 1 denotes the unit vector. By the Perron- Frobenius theory there is a unique positive right eigenvector r associated with the eigenvalue ρ and we can normalize to get

$$\bar{p}_i = {}^{r_i}/_{\sum_{i=1}^{3} r_i}.$$

Since $(P + \rho E)\bar{p} = \rho\bar{p}$, then $P\bar{p} = 0$ and $\bar{p} > 0$. By the Perron-Frobenius theorem we get, (see Akin (1979) that the matrix P is a stable matrix on S, i.e. P has one zero eigenvalue and the other eigenvalues have negative real parts. This proves the statement of the proposition. It follows that system (10) has a unique positive equilibrium $\bar{p}$ with entries

$$\bar{p}_1(I) = \frac{\beta\delta I + \gamma\delta}{F} \qquad (12)$$
$$\bar{p}_2(I) = \frac{\alpha\delta I}{F}$$
$$\bar{p}_3(I) = \frac{\alpha\beta I^2}{F},$$

where $F = \alpha\beta I^2 + (\alpha + \beta)\delta I + \gamma\delta$.

The simplex S is positively invariant. System (10) for all $I \geq 0$ has a unique positive equilibrium $\bar{p}(I)$ with entries given by (12).
The equilibrium $\bar{p}(I)$ is globally asymptotically stable on S, that means for fixed light intensity I all solutions with initial condition $p(0) \in S$ converge to $\bar{p}(I)$.

4.3. Optimization of Photosynthetic Production
Let us assume that phytoplankton regulates its photosynthetic production rate (FP) with a certain strategy which maximizes production. The rate of the photosynthetic production FP is proportional to the number of transitions from x_2 to x_1. Let us investigate the optimal values of light intensity $I(t)$, for which the photosynthetic production $FP = \gamma p_2(t)$ is maximal under constraints $I \in [I_{min}, I_{max}]$.
We will examine two strategies:
1. Instantaneous maximal photosynthetic production with respect to I, (local optimality), i.e.

$$\dot{p}_2 = f_2(p, I, t) \rightarrow max$$

for all t, under the constraints $I \in [I_{min}, I_{max}]$.
2. Integral maximal biomass (global optimality), i.e.

$$J(I) = \int_0^{t_f} \gamma p_2(t) dt,$$

under the constraints $I \in [I_{min}, I_{max}]$.

4.4. Local Optimality
In the case of strategy 1, we maximize the following function:

$$J\big(I(t)\big) = I(t)\alpha p_1(t) - I(t)\beta p_2(t)$$

under the constraints $I \in [I_{min}, I_{max}]$. For $p(t) = \bar{p}(I)$ we examine the following function:

$$FP(I) = \frac{\alpha\delta I\gamma}{\delta\gamma + (\beta\delta + \alpha\delta)I + \alpha\beta I^2}.$$

By straightforward calculation we get that the optimal light intensity is given by

$$I^* = \sqrt{\frac{\gamma\delta}{\alpha\beta}}.$$

4.5. Global Optimality
In case of strategy 2, we have the following optimal control problem: Find a function $\hat{I}(t)$ for which the goal function

$$J(I) = \int_0^{t_f} \gamma p2(t)\, dt$$

attains its maximum, where t_f is fixed. We introduce an additional state variable

$$p_0(t) = \int_0^t \gamma p_2(s) ds \qquad (13)$$

defined by

$$\dot{p_0}(t) = \gamma p_2(t), \qquad p_0(0) = 0.$$

We are led to the following optimal control problems:

$$Maximize\ p_0\big(t_f\big) \qquad (14)$$

under the constraints

$$c_1(p, I) = I_{min} - I \leq 0$$
$$c_2(p, I) = I - I_{max} \leq 0.$$

Discretization of Eqs. (10, 13, 14) using Eqs. (6, 7, 8) and state equation (4) leads to

$$Minimize\ \left(-p_0^N\right)$$

subject to
$$p^{i+1} = p^i + hf(p^i, I^i), \qquad i = 0, \dots, N-1,$$

$\lambda_i = \lambda^{i+1} + h\lambda^{i+1} f_{x^i}(x^i, u^i) + \mu^i c_{x^i}(x^i, u^i),$
$i = N-1, \ldots, 0,$

$\lambda_0^i = -1, \qquad i = 0, \ldots, N-1,$

$\lambda^N = (-1, 0, 0, 0),$

$0 = h\lambda^{i+1} f_{I^i}(p^i, I^i) + \mu^i c_{I^i}(p^i, I^i),$

where the vector function

$F(p, I) = (-\gamma p_2, f_1(p, I), \ldots, f_3(p, I))$

is given by Eq. (13) and by right-hand side of Eq. (10). In the adaptive critic synthesis, the critic and action network were selected such that they consist of three and two subnetworks, respectively, each having 3-18-1 structure (i.e. three neurons in the input layer, eighteen neurons in the hidden layer and one neuron in the output layer).

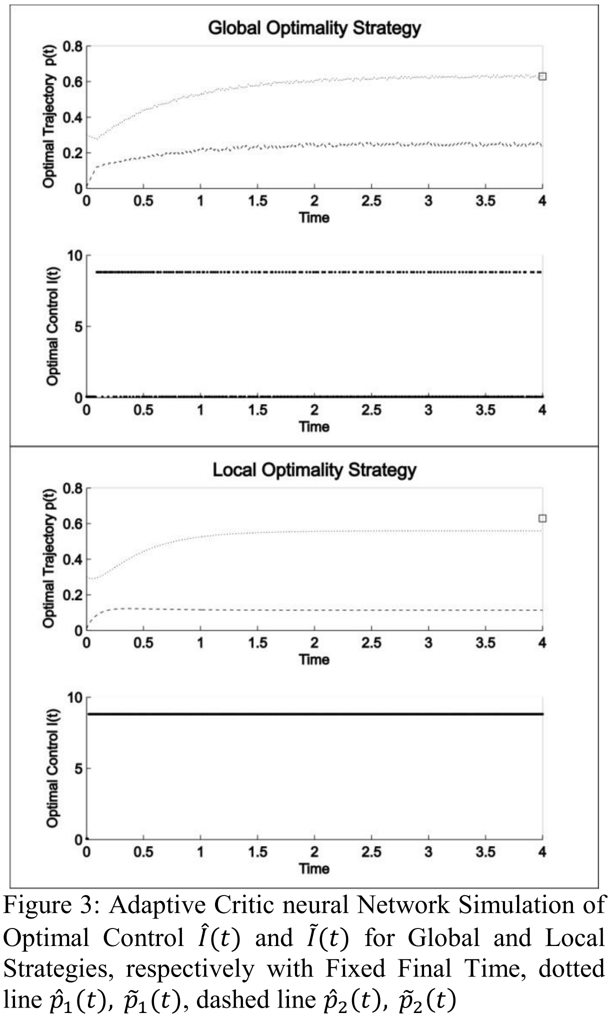

Figure 3: Adaptive Critic neural Network Simulation of Optimal Control $\hat{I}(t)$ and $\tilde{I}(t)$ for Global and Local Strategies, respectively with Fixed Final Time, dotted line $\hat{p}_1(t)$, $\tilde{p}_1(t)$, dashed line $\hat{p}_2(t)$, $\tilde{p}_2(t)$

The results of numerical solutions (Figure 3) have shown that the optimal strategies $\tilde{I}(t)$ and $\hat{I}(t)$ based on short or long-term perspective, respectively, have different time trajectory, for a given initial condition $\tilde{I}(t) = I_{max}$ and optimal control $\hat{I}(t)$ for long-term strategies obtains extreme values of the control set, i.e. optimal control is bang-bang. For long-term strategy optimal trajectory $\hat{p}_2(t)$ converges to $\bar{p}_2(I^*)$. Therefore let us consider the following free final time optimal control problems

$$J(t_f, I) = \int_0^{t_f} \gamma p_2(t) dt$$

and

$$J(t_f, I) = \int_0^{t_f} dt$$

with final condition $\psi(p(t_f)) = 0$, where $\psi(p) = (p_1 - \bar{p}_1(I^*), p_2 - \bar{p}_2(I^*))$. Results of adaptive-critic simulations are shown in Figure 4.

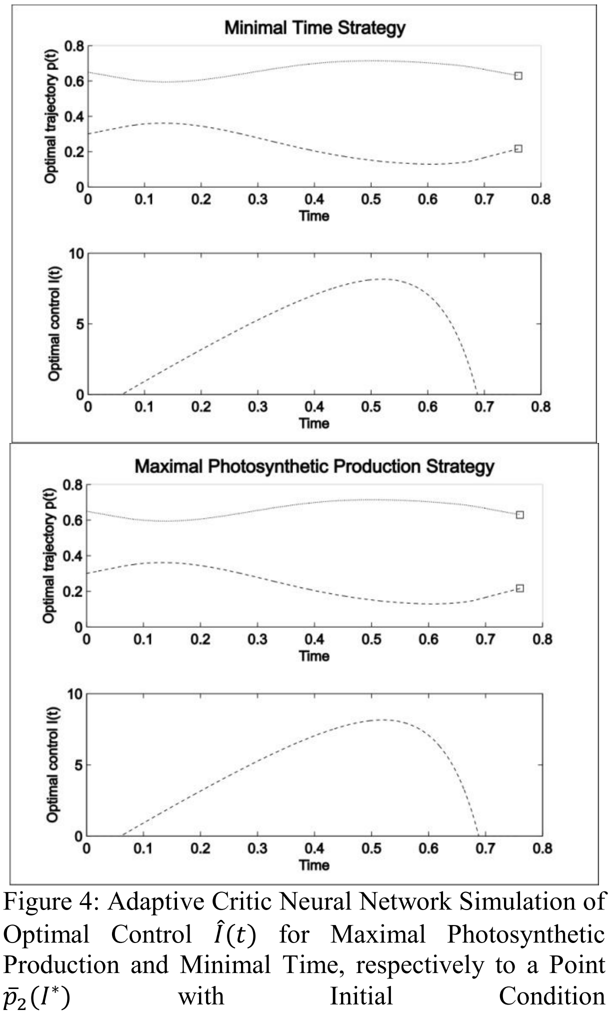

Figure 4: Adaptive Critic Neural Network Simulation of Optimal Control $\hat{I}(t)$ for Maximal Photosynthetic Production and Minimal Time, respectively to a Point $\bar{p}_2(I^*)$ with Initial Condition $x(0) = (0.3;\ 0.65;\ 0.05)$ (dotted line $\hat{p}_1(t)$, dashed line $\hat{p}_2(t)$)

The results of numerical calculations have shown that the proposed adaptive critic neural network is able to meet the convergence tolerance values that we choose, which led to satisfactory simulation results. Simulations, using MATLAB show that proposed neural network is able to solve nonlinear free final time optimal control problem with state and control constraints.

5. NITROGEN TRANSFORMATION CYCLE

5.1. Description of the Model

The aerobic transformation of nitrogen compounds (Kmet, 1996), (Kmet, 2009) includes:

- the decomposition of complex organic substances into simpler compounds, ammonium being the final nitrogen product,
- ammonium and nitrate oxidation,
- the assimilation of nitrates.

Specific groups of microorganisms participate in these processes. Heterotrophic bacteria (x_1) assimilates and decomposes the soluble organic nitrogen compounds DON x_6 derived from detritus x_5. Ammonium x_7, one of the final decomposition products undergoes a biological transformation into nitrate x_9. This is carried out by aerobic chemoautotrophic bacteria in two stages: ammonia is first oxidized by nitrifying bacteria from the genus Nitrosomonas x_2 into nitrites x_8 that serve as an energy source for nitrating bacteria mainly from the genus Nitrobacter x_3. The resulting nitrates may be assimilated together with ammonia and soluble organic forms of nitrogen by the phytoplankton x_4, whereby the aerobic transformation cycle of nitrogen compounds is formed (Figure 5).

The individual variables $x_1,\ldots,x_9$ represent nitrogen concentrations contained in the organic as well as in inorganic substances and living organisms presented in a model.

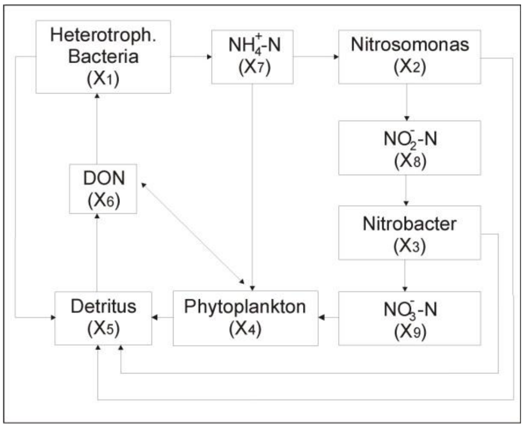

Figure 5: Diagram of the Compartmental System Modelled by Eq. (15)

The following system of ordinary differential equations is proposed as a model for the nitrogen transformation cycle:

$$\dot{x}_i = x_i(U_i(x) - E_i(x) - M_i(x))$$
$$\dot{x}_5 = \sum_{i=1}^{4} x_i M_i(x) - K_5 x_5$$
$$\dot{x}_6 = K_5 x_5 - x_1 U_1(x) + x_4 E_4(x) - x_4 P_6(x) \qquad (15)$$
$$\dot{x}_7 = x_1 E_1(x) - x_2 U_2(x) - x_4 P_7(x)$$
$$\dot{x}_8 = x_2 E_2(x) - x_3 U_3(x)$$
$$\dot{x}_9 = x_3 E_3(x) - x_4 P_9(x)$$

where x_i are the concentration of the recycling matter in microorganisms, the available nutrients and detritus, respectively (15).

$$U_i(x) = \frac{K_i x_{i+5}}{1 + g_i x_{i+5}} \quad \text{for } i = 1,2,3,4$$
$$p = u_1 x_6 + u_2 x_7 + u_3 x_9$$

$$U_4(x) = \frac{K_4 p}{1 + g_4 p}\ , \quad U - \text{uptake rate}$$

$$L_i(x) = \frac{a_{2i-1} U_i(x)}{1 + a_{2i} U_i(x)} + 1 - \frac{a_{2i-1}}{a_{2i}},$$
$$L - \text{excretion activity}$$

$$M_i(x) = g_{2i+3} + g_{2i+4} L_i(x), \qquad M - \text{mortality rate}$$

$$E_i(x) = U_i(x) L_i(x) \quad \text{for } i = 1,2,3,4,$$
$$E - \text{excretion rate}$$

$$P_i(x) = \frac{K_4 u_i x_i}{1+g_4 p} \quad \text{for } i = 6,7,9.$$

5.2. Optimal Biomass Production

The variables $u = (u_1, u_2, u_3)$ express the preference coefficients for update of x_6, x_7, x_9. It can be expected that the phytoplankton will employ control mechanisms in such a way as to maximize its biomass over a given period *T* of time:

$$J(u) = \int_0^{t_f} x_4(t)dt \ \rightarrow max$$

under the constraints

$$c(x,u) := b_1 U_4(x,u) + b_2 P_6(x,u) + b_3 P_9(x,u) + b_4 E_4(x,u) \le W(I),$$

$u_i \in [0, u_{i\,max}]$ for $i = 1,2,3.$

The last inequality expresses the fact that amount of energy used for ”living expenses” (synthesis, reduction and excretion of nutrients) by phytoplankton cannot exceed a certain value *W*(*I*) which depends on light intensity I (for detail explanation see (Kmet, 1996)). We introduce an additional state variable

$$x_0(t) = \int_0^t x_4(s)ds \qquad (16)$$

defined by

$$\dot{x}_0(t) = x_4(t), x_0(0).$$

We are led to the following optimal control problems:

1) long-therm strategy:

$$Maximize\ x_0(t_f) \tag{17}$$

under the constrains

$$c(x,u) \le W(I),\ \ u_i \in [0, u_{i\,max}]\ for\ i = 1,2,3.$$

2) short-therm strategy:

$$Maximize\ f_4(x,u) = U_4(x,u) - E_4(x,u) - M_4(x,u)$$

for all $t \in [t_0, t_f]$ under the constrains

$$c(x,u) \le W(I),\ \ u_i \in [0, u_{i\,max}]\ for\ i = 1,2,3.$$

Discretization of Eqs. (15 - 17) using Eqs. (6 - 8) and state equation (4) leads to

$$Minimize\ (-x_0^N) \tag{19}$$

subject to

$$x^{i+1} = x^i + hF(x^i, u^i), \qquad i = 0, \dots, N-1,$$

$$\lambda_i = \lambda^{i+1} + h\lambda^{i+1} F_{x^i}(x^i, u^i) + \mu^i c_{x^i}(x^i, u^i),$$
$$i = N-1, \dots, 0,$$

$$\lambda_0^i = -1, \qquad i = 0, \dots, N-1,$$

$$\lambda^N = (-1,0,0,0,0,0,0,0,0,0),$$

$$0 = h\lambda^{i+1} F_{u^i}(x^i, u^i) + \mu^i c_{u^i}(x^i, u^i),$$

where the vector function

$$F(x,u) = (-x_6, F_1(x,u), \dots, F_9(x,u))$$

is given by Eq. (16) and by right-hand side of Eq. (15).

The solution of optimal control with state and control constraints using adaptive critic neural network and NLP methods is displayed in Figs. 6 - 10 for different initial conditions $x(0)$ and different values of reduction coefficients b_2 and b_3. We used values of coefficients given in Table 1 for numerical calculation.

Table 1: Values of the Constants Used in the Model

$a_1 = 0.007$	$u_7 = 0.03$
$a_2 = 0.0182$	$u_9 = 0.2$
$a_3 = 0.5$	$g_1 = 0.14$
$a_4 = 0.67$	$g_2 = 1.5$
$a_5 = 1$	$g_3 = 2.0$
$a_6 = 1.39$	$g_4 = 1.5$
$a_7 = 0.66$	$g_5 = 0.8$
$a_8 = 0.67$	$g_6 = 0.4$
$K_1 = 19.3$	$g_7 = 0.2$
$K_2 = 8.17$	$g_8 = 0$
$K_3 = 71.28$	$g_9 = 0.15$
$K_4 = 3.4323$	$g_{10} = 0$
$K_5 = 0.62$	$g_{11} = 0.1$
$u_6 = 0.01$	$g_{12} = 0$

In the adaptive critic synthesis, the critic and adaptive network were selected such that they consist of nine and four subnetworks, respectively, each having 9-27-1 structure (i.e. nine neurons in the input layer, twenty-seven neurons in the hidden layer and one neuron in the output layer). The proposed adaptive critic neural network is able to meet the convergence tolerance values that we choose, which led to satisfactory simulation results. Simulation using MATLAB shows that there is a very good agreement between short-term and long-term strategy and proposed neural network is able to solve nonlinear optimal control problem with state and control constraints.

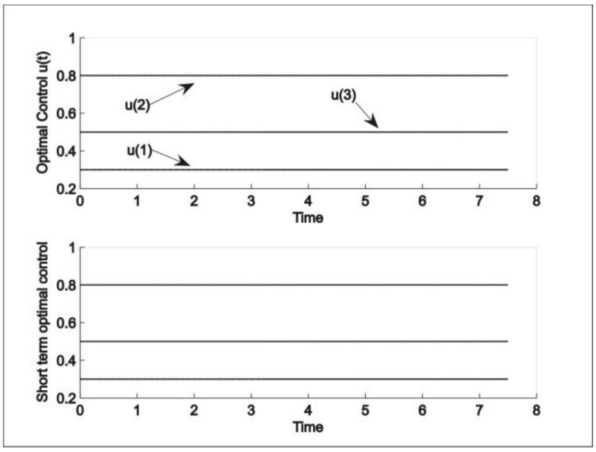

Figure 6: Adaptive Critic Neural Network Simulation of Optimal Control $\hat{u}(t)$ for Initial Condition $x(0) = (0.01,0.01,0.02,0.001,0.04,0.001,0.001,0.07,0.01)$ and $b_2 < b_3$ or $b_3 < b_2$

The optimal strategy is the following. In the presence of high ammonium concentration, the uptake of DON and nitrate is stopped. If the concentration of ammonium drops below a certain limit value, phytoplankton and long-term strategy and proposed neural network is able to solve nonlinear optimal control problem with state and control constraints. The optimal strategy is the following. In the presence of high ammonium concentration, the uptake of DON and nitrate is stopped. If the concentration of ammonium drops below a certain limit value, phytoplankton starts to assimilate DON or nitrate dependently on values b_2, b_3.

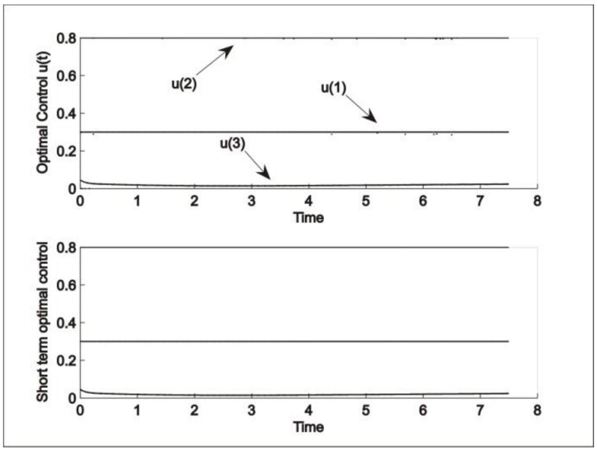

Figure 7: Adaptive Critic Neural Network Simulation of Optimal Control $\hat{u}(t)$ for Initial Condition $x(0) = (0.1,0.1,0.2,0.8,0.4,0.001,0.001,0.7,1)$ and $b_2 < b_3$

If the concentration of all three forms of nitrogen are low all of them are assimilated by phytoplankton at the maximal possible rate, i.e. $\hat{u}_i(t) = u_{imax}$ for all $t \in [t_0, t_f]$ (Figure 6). Our results are quite similar to those obtained by (Kmet, 1996).

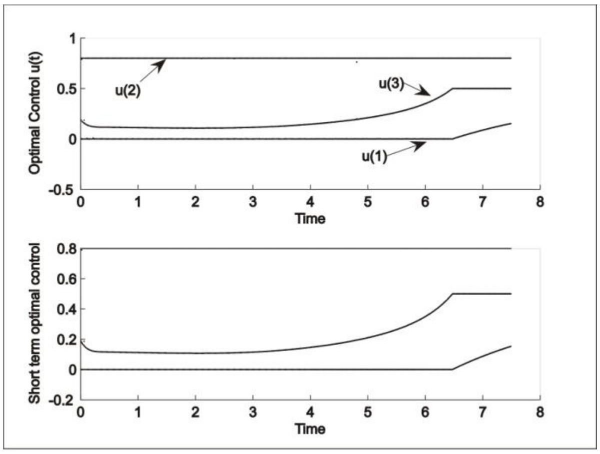

Figure 8: Adaptive Critic Neural Network Simulation of Optimal Control $\hat{u}(t)$ for Initial Condition $x(0) = (0.1,0.1,0.2,0.8,0.4,0.001,0.001,0.7,1)$ and $b_3 < b_2$

6. CONCLUSION

A single network adaptive critic approach is presented for optimal control synthesis with control and state constraints. We have formulated, analysed and solved an optimal control problems related to optimal photosynthetic production and optimal biomass production, respectively. Using MATLAB, a simple simulation model based on adaptive critic neural network was constructed. Numerical simulations have shown that adaptive critic neural network is able to solve nonlinear optimal control problem with control and state constraints and fixed and free final time.

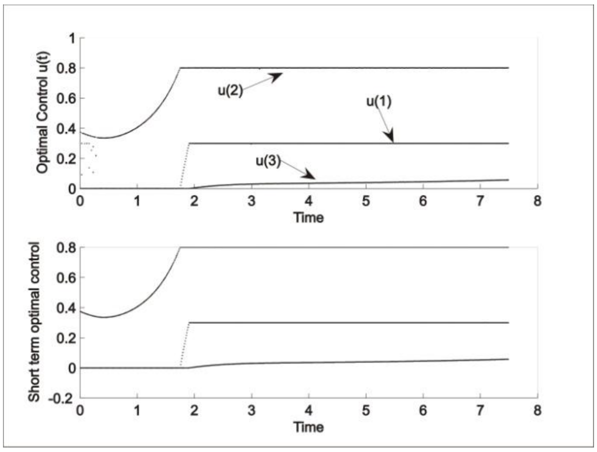

Figure 9: Adaptive Critic Neural Network Simulation of Optimal Control $\hat{u}(t)$ for Initial Condition $x(0) = (0.1,0.1,0.2,0.8,0.4,0.5,0.6,0.7,1)$ and $b_2 < b_3$

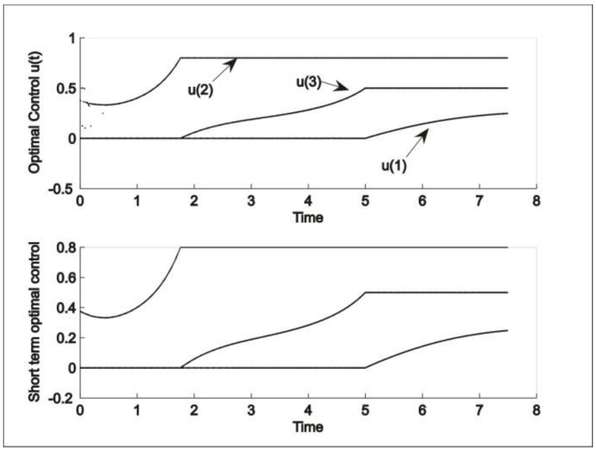

Figure 10: Adaptive Critic Neural Network Simulation of Optimal Control $\hat{u}(t)$ for Initial Condition $x(0) = (0.1,0.1,0.2,0.8,0.4,0.5,0.6,0.7,1)$ and $b_3 < b_2$

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