NEURAL NETWORK SIMULATION OF NITROGEN TRANSFORMATION CYCLE

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ABSTRACT

A neural network based optimal control synthesis is presented for solving optimal control problems with control and state constraints. The optimal control problem is transcribed into a nonlinear programming problem which is implemented with adaptive critic neural network. The proposed simulation method is illustrated by the optimal control problem of nitrogen transformation cycle model. Results show that adaptive critic based systematic approach holds promise for obtaining the optimal control with control and state constraints.

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 (Polak, 1997), (Kirk, 1998)) for solving a optimal control problem. Most of the literature that deals with numerical methods for the solution of general optimal control problems focuses on the 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 at al., 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 multi-layer feedforward neural networks have been used for obtaining numerical solutions to the optimal control problem. (Padhi at al., 2001), (Padhi et al., 2006). We have taken hyperbolic tangent sigmoid transfer function for the hidden layer and a linear transfer function for the output layer.

The paper extends adaptive critic neural network architecture proposed by (Padhi at al., 2001) to the optimal control problems with control and state constraints. The paper is organized as follows. In Section 2, the optimal control problems with control and state constraints are introduced. We summarize necessary optimality conditions and give a short overview of basic result including the iterative numerical methods. Section 3 discusses discretization methods for the given optimal control problem. It also discusses a form of the resulting $nonlinear\ programming\ problems$. Section 4 presents a short description of $adaptive\ critic\ neural\ network\ synthesis$ for optimal problem with state and control constraints. Section 5 consists of a nitrogen transformation model. In section 6, we apply the discussed methods to the nitrogen transformation cycle. The goal is to compare short-term and long-term strategies of assimilation of nitrogen compounds. Conclusions are presented in Section 7.

OPTIMAL CONTROL PROBLEM

We consider a 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

$$F(x,u) = g(x(t_f)) + \int_{t_0}^{t_f} f_0(x(t), u(t))dt \quad (1)$$

subject to

$$\begin{aligned} \dot{x}(t) &= f(x(t), u(t)), \\ x(t_0) &= x_0, \\ \psi(x(t_f)) &= 0, \\ c(x(t), u(t)) &\leq 0, \ \ t \in [t_0, t_f]. \end{aligned}$$

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 $\psi : R^{n+m} \to R^r$, $0 \leq r \leq n$ 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 (cf. (Pontryagin at al., 1983), (Kirk, 1998)).

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We introduce an additional state variable

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

defined by the

$$\dot{x}_0(t) = f_0(x(t), u(t)),\ x_0(0) = 0.$$

Then the $augmented\ Hamiltonian\ function$ for problem (1) is

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

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) (cf. (Kirk, 1998), (Pontryagin at al., 1983)) implies that there exist a piecewise continuous and piecewise continuously differentiable $adjoint\ function\ \lambda : [t_0, t_f] \rightarrow R^{n+1}$, a piecewise continuous $multiplier\ function\ \mu : [t_0, t_f] \rightarrow R^q,\ \mu(t) \geq 0$ and a multiplier $\sigma \in R^r$ satisfying

$$\begin{aligned} \dot{\lambda}_j(t) &= -\frac{\partial H}{\partial x_j}(\hat{x}(t), \lambda(t), \mu(t), \hat{u}(t)) \\ \lambda_j(t_f) &= g_{x_j}(\hat{x}(t_f)) + \sigma\psi_{x_j}(\hat{x}(t_f)) \\ & \quad j = 0, \ldots, n \\ \dot{\lambda}_0(t) &= 0 \\ 0 &= \frac{\partial H}{\partial u}(\hat{x}(t), \lambda(t), \mu(t), \hat{u}(t)). \end{aligned} \quad (3)$$

Herein, the subscript x or u denotes the partial derivative with respect to x or u.

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 $t_i \in [t_0, t_f],\ i = 0, \ldots, N$, be a equidistant mesh point with $t_i = t_0 + ih, i = 1, \ldots, N$, where $h = \frac{t_f - t_0}{N}$. Let the vectors $x^i \in R^{n+1},\ u^i \in R^m, i = 1, \ldots, N$, 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

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

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

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

where

$$G(x^N) = g((x_1, \ldots, x_n)^N) + x_0^N,$$

subject to

$$\begin{aligned} -x^{i+1} + x^i + hf(x^i, u^i) &= 0, \quad (4) \\ x^0 &= x(t_0) \\ \psi(x^N)) &= 0, \\ c(x^i, u^i) &\leq 0, \\ i &= 0, \ldots, N-1. \end{aligned}$$

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

$$\begin{aligned} L(z, \lambda, \sigma, \mu) &= \sum_{i=0}^{N-1} \lambda^{i+1}(-x^{i+1} + x^i + hf(x^i, u^i) \\ &+ G(x^N) + \sigma\psi(x^N) + \\ & \sum_{i=0}^{N-1} \mu^i c(x^i, u^i). \end{aligned} \quad (5)$$

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

$$\begin{aligned} 0 = L_{x^i}(s, \lambda, \mu) &= \lambda^{i+1} + h\lambda^{i+1} f_{x^i}(x^i, u^i) - \\ & \lambda^i + \mu^i c_{x^i}(x^i, u^i), \quad (6) \\ & i = 0, \ldots, N-1, \\ 0 = L_{x^N}(s, \lambda, \mu) &= G_{x^N}(x^N) + \quad (7) \\ & \sigma\psi_{x_N}(x_N) - \lambda^N, \\ 0 = L_{u^i}(s, \lambda, \mu) &= h\lambda^{i+1} f_{u^i}(x^i, u^i) \\ & + \mu^i c_{u^i}(x^i, u^i), \quad (8) \\ & i = 0, \ldots, N-1. \end{aligned}$$

Eq. $(6-8)$ represents the discrete version of necessary condition (3) for optimal control problem (1).

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, et al.,1989), (Sandberg, 1998). Neurons are grouped into distinct layers and interconnected according to a given architecture Fig. (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

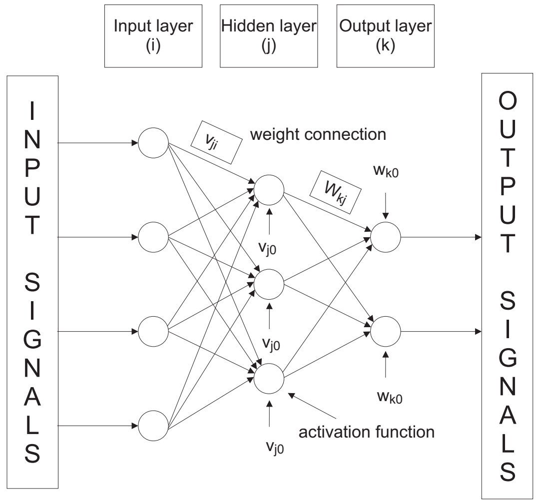

Figure 1: Feed forward neural network topology with one hidden layer, $v_{ji},\ w_{kj}$ are values of connection weights, $v_{j0},\ w_{k0}$ are values of bias

forward network often has one or more hidden layers of sigmoid neurons followed by an output layer of linear neurons.

Fig. (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 $in = [in_1, \ldots, in_{n_i}]$ and $out = [out_1, \ldots, out_{n_o}]$ be the input and output vectors of the network, respectively. Let $V = [v_1, \ldots, v_{n_{hl}}]$ be the matrix of synaptic weights between the input nodes and the hidden units, where $v_j = [v_{j0}, v_{j1} \ldots, v_{jn_i}]$, v_{j0} is the bias of the jth hidden unit, and v_{ji} is the weight that connects the ith input node to the jth hidden unit.

Let also $W = [w_1, \ldots, w_{n_o}]$ be the matrix of synaptic weights between the hidden and output units, where $w_k = [w_{k0}, w_{k1} \ldots, w_{kn_o}]$, w_{k0} is the bias of the kth output unit, and w_{kj} is the weight that connects the jth hidden units to the kth output unit.

The response of the jth hidden unit is given by

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

where $tanh(.)$ is the activation function for the hidden units. The response of the kth 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.

The multi-layered feed forward network shown in Fig. (2) is training using the steepest descent error backpropagation rule. Basically, it is a gradient descent, parallel

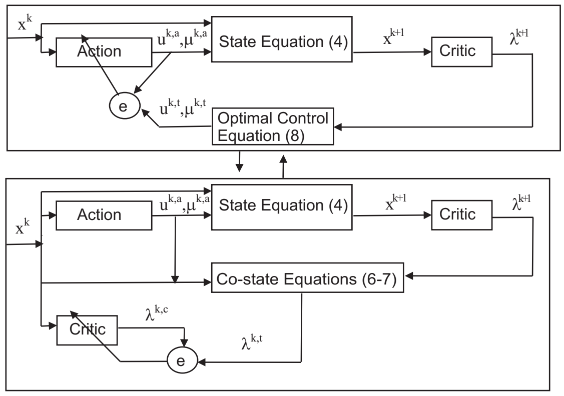

Figure 2: Architecture of adaptive critic network synthesis

distributed optimization technique to minimise the error between the network and the target output (Rumelhart at al., 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 network 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 at al., 1987).

From free terminal condition ($\psi(x) \equiv 0$) and from Eqs. (6-7) we obtain that $\lambda_0^i = -1,\ for\ i = N, \ldots, 0\ and\ \lambda_j^N = 0,\ for\ j = 1, \ldots, n.$ We use this observation before proceeding to the actual training of the *adaptive critic neural network*. The training process of the adaptive critic networks is carried out in the following steps. For $i = 1, \ldots, I$ define the sets $S_i = \{x^k \in R^{n+1} : ||x^k|| < s_i\}$, where $||.||$ denotes the Euclidean norm and s_i is a positive constant. The netwoks are trained for states within S_i. After convergence we choose $s_{i+1} > s_i$, set S_{i+1} and training the networks until $i = I - 1$.

The steps for training the action network are as follows: When

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

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:

When

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

1) Generate set S_i. For all $x^k \in S_i$, 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 and λ^{k+1} solve (8) to calculate $u^{k,t}$ and $\mu^{k,t}$.

1) Generate set S_i. For all $x^k \in S_i$, 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 $\lambda^{k,c}$.

the convergence criterion for the critic network training is met.

Further discussion and detail explanation of this adaptive critic methods can be found in (Padhi at al., 2001), (Padhi et al., 2006).

NITROGEN TRANSFORMATION CYCLE

The aerobic transformation of nitrogen compounds (Kmet, 1996) 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 Fig. (3). 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.

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

$$\begin{aligned}
\dot{x}_i(t) &= x_i(t)U_i(x(t)) \\
&\quad -x_i(t)E_i(x(t)) - x_i(t)M_i(x(t))) \\
\dot{x}_5(t) &= \sum_{i=1}^{4} x_i M_i(x) - K_5 x_5(t) \\
\dot{x}_6(t) &= K_5 x_5(t) - x_1(t)U_1(x(t)) + \\
&\quad x_4(t)E_4(x(t)) - x_4(t)P_6(x(t)) \\
\dot{x}_7(t) &= x_1(t)E_1(x(t)) - \\
&\quad x_2(t)U_2(x(t)) - x_4(t)P_7(x(t)) \\
\dot{x}_8(t) &= x_2(t)E_2(x(t)) - x_3(t)U_3(x(t)) \\
\dot{x}_9(t) &= x_3(t)E_3(x(t)) - x_4(t)P_9(x(t))
\end{aligned} \tag{9}$$

where $x_i(t)$ are the concentration of the recycling matter in microorganisms, the available nutrients and detritus, respectively (9).

$$\begin{aligned}
U_i(x) &= \tfrac{K_i x_{i+5}}{1+g_i x_{i+5}} \qquad for\ i = 1,2,3,4 \\
p &= u_1 x_6 + u_2 x_7 + u_3 x_9 \\
U_4(x) &= \tfrac{K_4 p}{1+g_4 p} \\
&\quad U - uptake\ rate \\
L_i(x) &= \tfrac{a_{2i-1}U_i(x)}{1+a_{2i}U_i(x)} + 1 - \tfrac{a_{2i-1}}{a_{2i}} \\
&\quad L - excretion\ activity \\
M_i(x) &= g_{2i+3} + g_{2i+4} L_i(x) \\
&\quad M - mortality\ rate \\
E_i(x) &= U_i(x)L_i(x) \qquad for\ i = 1,2,3,4 \\
&\quad E - excretionrate \\
P_i(x) &= \tfrac{K_4 u_i x_i}{1+g_4 p} \qquad for\ i = 6,7,9.
\end{aligned}$$

Three 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:

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

under the constraints

$$\begin{aligned}
c(x,u) &:= b_1 U_4(x,u) + \\
b_2 P_6(x,u) &+ b_3 P_9(x,u) + \\
b_4 E_4(x,u) &\leq W(I), \\
u_i &\in [0, u_{imax}]\ for\ i = 1,2,3.
\end{aligned}$$

The last inequality expresses the fact that amount of energy used for "living expenses" (synthesis, reduction and

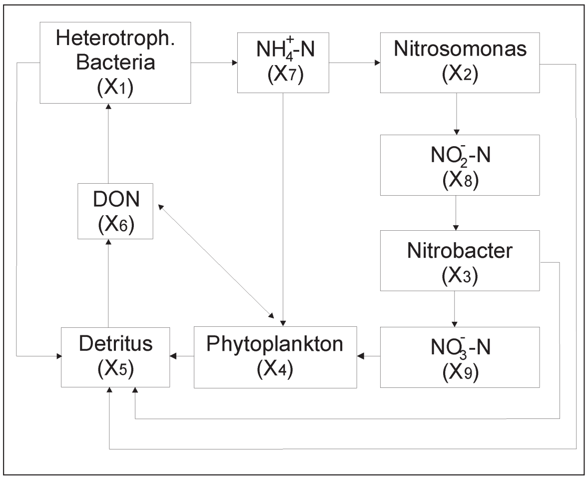

Figure 3: Diagram of the compartmental system modelled by Eq. (9)

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

$$x_0(t) \quad = \quad \int_0^t x_4(s)ds \tag{10}$$

defined by the

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

We are led to the following optimal control problems:

1) long-therm strategy:

$$Maximize\, x_0(t_f) \tag{11}$$

under the constraints

$$\begin{aligned} c(x,u) &\leq W(I), \\ u_i &\in [0, u_{imax}] \ for\ i = 1,2,3. \end{aligned} \tag{12}$$

2) short-therm strategy:

$$\begin{aligned} &Maximize \\ &f_4(x,u) = U_4(x,u) - E_4(x,u) - M_4(x,u) \end{aligned}$$

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

$$\begin{aligned} c(x,u) &\leq W(I), \\ u_i &\in [0, u_{imax}] \ for\ i = 1,2,3. \end{aligned}$$

Discretization of Eqs. (9 - 11) using Eqs. (6- 8) and state equation (4) leads to

$$Minimize \quad -x_0^N \tag{13}$$

subject to

$$\begin{aligned} x^{i+1} &= x^i + hF(x^i, u^i) \\ & \quad i = 0, \dots, N-1, \\ \lambda^i &= \lambda^{i+1} + h\lambda^{i+1} F_{x^i}(x^i, u^i) \\ & \quad +\mu^i c_{x^i}(x^i, u^i), \qquad (14) \\ & \quad i = N-1, \dots, 0, \\ \lambda_0^i &= -1,\ i = 0, \dots, N-1 \\ \lambda^N &= (-1, 0, 0, 0, 0, 0, 0, 0, 0, 0), \qquad (15) \\ 0 &= h\lambda^{i+1} F_{u^i}(x^i, u^i) \\ & \quad +\mu^i c_{u^i}(x^i, u^i), \qquad (16) \end{aligned}$$

where the vector function

$$F(x,u) \quad = \quad (-x_4, F_1(x,u), \dots, F_9(x,u))$$

is given by Eq. (10) and by right-hand side of Eq. (9).

NUMERICAL SIMULATION

The solution of optimal control with state and control constraints using $adaptive\ critic\ neural\ network$ and NLP methods is displayed in Figs. (4 - 8) for different initial conditions $x(0)$ and different values of reduction coefficients b_2 and b_3. We used values of coefficients given in Tab. (1) for numerical calculation. 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. Simulations, using MATLAB show 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. The optimal strategy is the following. In the presence of high ammonium concentration, the uptake of DON and nitrate

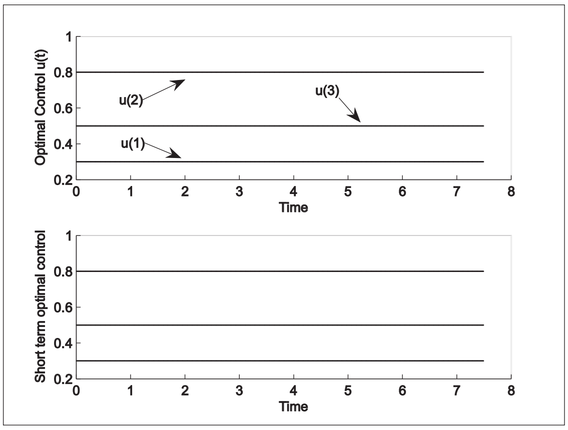

Figure 4: Adaptive critic neural network simulation of optimal control $\hat{u}(t)$ for initial condition $x(0) = (0.01, 0.01, 0.02, 0.001, 0.04, 0.001, .001, 0.07, 0.01)$ and $b_2 < b_3$ or $b_3 < b_2$

is stopped. If the concentration of ammonium drops below a certain limit value, phytoplankton starts to assimilate DON or nitrate dependently on values $b_2,\ b_3$. If the concentration of all three forms of nitrogen are low, all of them are assimilated by phytoplankton at the maximal possible rate, e.i. $\hat{u}_i(t) = u_{imax}$ for all $t \in [t_0, t_f]$ (Fig. 4). Our results are quite similar to those obtained by (Kmet, 1996).

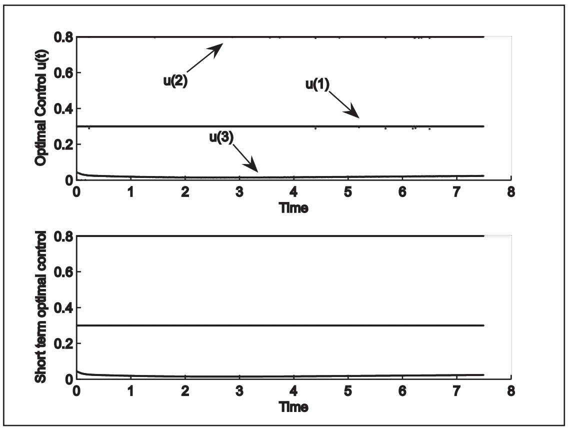

Figure 5: Adaptive critic neural network simulation of optimal control $\hat{u}(t)$ for initial condition $x(0) = (0.1, 0.1, 0.2, 0.8, 0.4, 0.001, .001, 0.7, 1.)$ and $b_2 < b_3$

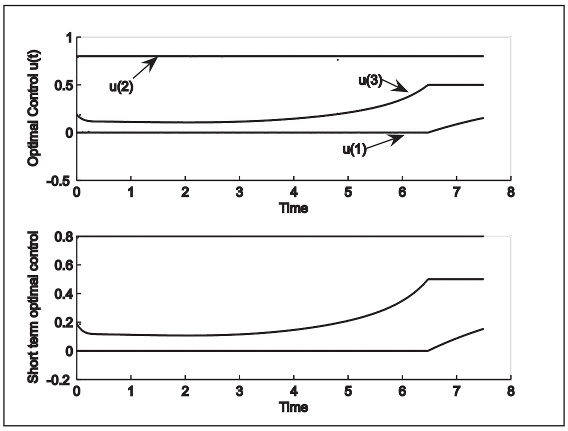

Figure 6: Adaptive critic neural network simulation of optimal control $\hat{u}(t)$ for initial condition $x(0) = (0.1, 0.1, 0.2, 0.8, 0.4, 0.001, .001, 0.7, 1.)$ and $b_3 < b_2$

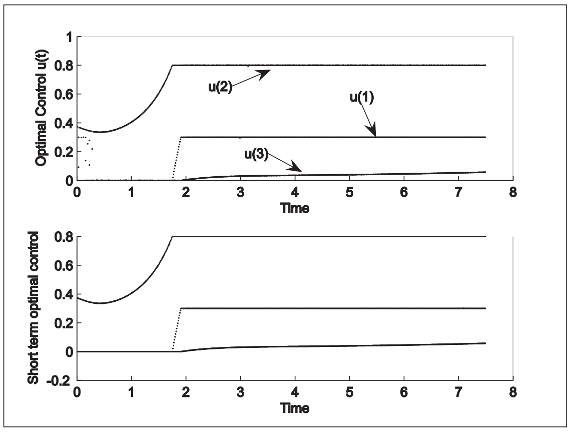

Figure 7: Adaptive critic neural network simulation of optimal control $\hat{u}(t)$ for initial condition $x(0) = (0.1, 0.1, 0.2, 0.8, 0.4, 0.5, 0.6, 0.7, .1)$ and $b_2 < b_3$

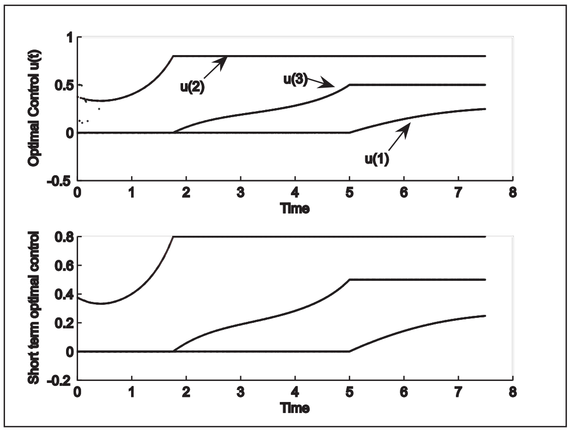

Figure 8: Adaptive critic neural network simulation of optimal control $\hat{u}(t)$ for initial condition $x(0) = (0.1, 0.1, 0.2, 0.8, 0.4, 0.5, 0.6, 0.7, .1)$ and $b_3 < b_2$

CONCLUSION

A new 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 problem related to optimal uptake of nutrient by phytoplankton. 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 it explains nutrient uptake by phytoplankton.

*

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APPENDIX

Table I. Values of the constants used in the model

$a_1 = 0.007$	$K_4 = 1.$
$a_2 = 0.0182$	$K_5 = 0.62$
$a_3 = 0.5$	$g_1 = 0.14$
$a_4 = 0.67$	$g_2 = 1.5$
$a_5 = 1.$	$g_3 = 2.0$
$a_6 = 1.39$	$g_4 = 1.5$
$a_7 = 0.66$	$g_5 = 0.8$
$a_8 = 0.67$	$g_6 = 0.4$
$b_1 = 2.92$	$g_7 = 0.2$
$b_2 = 0.4$ (9.0)	$g_8 = 0.$
$b_3 = 4.2$ (0.4)	$g_9 = 0.15$
$b_4 = 1.0$	$g_{10} = 0.$
$W(I) = 0.51$	$g_{11} = 0.1$
h=0.05	$g_{12} = 0.$
$K_1 = 19.3$	$\epsilon_a = 0.0001$
$K_2 = 8.17$	$\epsilon_c = 0.05$
$K_3 = 71.28$	$u_{1max} = 0.3$
$u_{2max} = 0.8$	$u_{3max} = 0.5$

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