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REAL-TIME OPTIMIZATION WITH ADAPTIVE VELOCITY ESTIMATOR AND APPLICATION TO SIGNAL SEPARATION OF CELL OSCILLATORS

Haruo Suemitsu, Shohei Ueno, Tadashi Konishi and Takami Matsuo*

Department of Mechatronics
Oita University
700 Dannoharu, Oita 870-1192, Japan
{ suemitu; ueno-shohei }@oita-u.ac.jp; konishi0874@me.com
*Corresponding author: matsuo@oita-u.ac.jp

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Abstract. *This paper extends the momentum method using an adaptive differential filter to the measurement-based optimization of an objective function with multivariable decision variables. The proposed method is a model-free real-time optimization algorithm with switching. Further, we define the signal separation problem from the dynamics of multi-cells to that of a single cell based on the assumption that the sum of the CO_2 uptakes of a crassulacean acid metabolism plant is a linear combination of delayed oscillation waves of cells. We apply the proposed momentum method to estimating delay sequences of CO_2 uptakes. Finally, we perform simulations using MATLAB/Simulink to verify the proposed method.*
Keywords: Crassulacean acid metabolism, Switching optimizer, Momentum optimization method

1. **Introduction.** In biological plants, the circadian rhythms play important roles in gene expressions, photosynthesis, growth, and many other physiological processes. The plant circadian rhythm is composed of many self-sustained oscillations that synchronize with each other. Precise and ecological control of the circadian rhythm provides a key technology for enhancing the plant growth in a closed cultivation system where light-dark cycles change within a 24-h period [1]. Climatic extremes are currently threatening agricultural sustainability all over the world. CAM (Crassulacean Acid Metabolism) plants show remarkable metabolic plasticity for modulating nocturnal and diurnal CO_2 uptake and have been identified as competitive biomass accumulators compared to many C3 and C4 crops. One approach to increasing plant water-use efficiency is to introduce CAM into C3 crops [2]. Computational modeling of CAM accelerates the improvement of CAM crops in terms of biomass productivity and quality-related attributes [3]. Although a complex mathematical model of plants is combined with the integration of experimental data for gene expression, protein abundance, metabolite concentration, a modeling process is a complicated task. It is necessary to simplify the model for control design by using metabolic processes. Blasius et al. investigated the mechanism of endogenous circadian photosynthesis oscillations of plants performing CAM in terms of a nonlinear theoretical model [4, 5]. The model showed regular endogenous limit cycle oscillations that were stable for a wide range of temperatures, in a manner that complies well with experimental data. The nonlinear dynamical model of CAM can be discussed from the control theoretical viewpoint. The state-variables of the nonlinear dynamic equations denote an internal CO_2 concentration, a malate concentration in the cytoplasm, a malate concentration in the vacuole, and an order of the tonoplast membrane. The input variables are as follows:

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an external CO_2 concentration, a light intensity, and temperature. A dynamic estimator of the tonoplast order and a fuzzy identifier of the nonlinear function in the dynamics of the tonoplast order have been proposed [6]. Further, the frequency and phase-shift controllers were proposed using an external CO_2 concentration and light intensity as inputs [7]. Although these estimators and controllers require information on the state variables of a single cell, they are not directly measurable. Thus, we proposed a reconstruction method of the internal states of a single cell by using the CO_2 uptake from outside as the measurement data. The sum of the CO_2 uptake of all cells can be measured; however, the CO_2 uptake for each cell cannot be measured. The information about the states of each cell is required to control the plant rhythm. Thus, these states need to be estimated using a real-time optimization method based on the whole CO_2 uptakes as the available measurements. Kawasaki et al. introduced a model of the sum of the CO_2 uptakes as a linear combination of delayed oscillation waves of cells [8]. By using the model, the CO_2 uptake for each cell should separate from whole CO_2 uptakes that are collected online using a CO_2 analyzer. Thus, the parameter estimation problem of delayed oscillation waves of cells is formulated as a real-time optimization with multivariable decision variables. By solving this problem, a control of the plant biological rhythms becomes possible. Kawasaki et al. extended the momentum method of the gradient descent algorithm for a single variable to a real-time optimization application case by using the adaptive differential filter to estimate delay sequences of the CO_2 uptake [8]. The proposed method was calculating the ratio of the time-derivative of the objective function and that of the decision function as the gradient. This method is valid for a single decision variable even if the objective function is multimodal. However, there are several decision parameters in the separation of the delayed oscillation waves in CAM plants. The previous paper [8] presents an instance of a signal separation simulated using two optimizers of a single decision parameter when the number of the decision parameters was two. The second optimizer used the measurement data with a short delay to avoid interfering the first optimizer. However, the calculated values of the objective function and the decision variables did not converge.

In this paper, the momentum method using the adaptive differential filter is extended for a measurement-based optimization of an objective function with multivariable decision variables. Thus, we propose a switching optimizer with single variable optimizers to obtain the partial derivatives of the objective function. To evaluate the performance of the switching optimizer, we perform a numerical simulation of a time-varying quadratic objective function in two decision variables. Finally, we apply the proposed switching optimizer to the signal separation problem of the CAM plant. Our main contribution in this paper is to propose a switching law that allows us to apply the adaptive velocity estimator to estimating a gradient with respect to multiple decision variables. The simulation results of the time-varying quadratic objective function and the signal separation problem of the CO_2 uptake show the switching optimizer converges to the optimal decision parameters.

This paper is organized as follows. Section 2 introduces the switching momentum optimizer using the adaptive velocity estimator. Section 3 defines the signal separation problem of CAM plants and applies the momentum optimizer to the problem. Conclusions are given in Section 4.

2. **Momentum Method in Optimization Using Velocity Estimator.** RTO (Real-Time Optimization) is a category of closed-loop control that aims at optimizing process performance in real time for systems. The CO_2 analyzer can measure the whole CO_2 uptake. We estimate the parameters of the whole CO_2 uptake by using RTO method. Particularly, we propose a gradient descent method with momentum applicable to RTO by replacing the gradient of an objective function with respect to a decision variable with

a ratio of the time derivatives of the objective function and the decision variable. The time derivatives are estimated by using the adaptive velocity estimator [9, 10].

2.1. **Gradient calculation.** If the decision parameter, $d(t)$, is single and a function of time, the gradient of the objective function, $f(d(t))$ with respect to the decision variable can be written as

$$f'(d(t)) = \frac{\dot{f}(d(t))}{\dot{d}(t)} \tag{1}$$

where $f'(d(t))$ denotes a derivative of $f(d)$ with respect to d, and $\dot{f}(d(t))$ and $\dot{d}(t)$ denote derivatives with respect to t, respectively. This equation allows us to estimate the gradient in real time by using the time derivatives of data sequences.

2.2. **Adaptive velocity estimator.** We have proposed an adaptive observer for estimating the time-derivatives whose upper bounds are known [9, 10].

The estimate, $\hat{\dot{f}}(t) = \hat{\theta}_1(t)$, of the derivative of the signal $f(t)$ is given by the following adaptive observer and the update laws:

$$\dot{\hat{f}}(t) = -k\left(\hat{f}(t) - f(t)\right) + \hat{\theta}_1(t) - \hat{\epsilon}(t)\,\mathrm{sgn}\left(\hat{f}(t) - f(t)\right) \tag{2}$$

where $\hat{f}(t)$ is an estimate of $f(t)$, k denotes a positive constant parameter, and $\hat{\theta}_1(t)$ and $\hat{\epsilon}(t)$ denote adjustable parameters derived by the following update laws:

$$\dot{\hat{\theta}}_1(t) = -\gamma_1\left(\hat{f}(t) - f(t)\right) \tag{3}$$

$$\dot{\hat{\epsilon}}(t) = \left|\hat{f}(t) - f(t)\right| \tag{4}$$

where γ_1 denotes a positive constant. The estimate of $\dot{f}(t)$ is given by

$$\hat{\dot{f}} = \hat{\theta}_1(t) = -\int_0^t \gamma_1\left(\hat{f}(\tau) - f(\tau)\right)d\tau \tag{5}$$

We refer to this estimator as the adaptive velocity estimator.

2.3. **Momentum method in RTO.** By defining $f \in R$ as the objective function and $d \in R$ as a decision variable, the continuous-time momentum gradient descent [8] for searching a minimum of the objective function is given by

$$\ddot{d}(t) + a\dot{d}(t) = c\nabla f(d(t)) = cf'(d(t)) \tag{6}$$

where $f'(d(t))$ denotes the first order derivative of $f(d)$ with respect to d, $\dot{d}(t)$ and $\ddot{d}(t)$ denote the first order and second order derivatives of $d(t)$ with respect to time t, respectively. The constant parameters a and c denote the momentum coefficient and the learning rate, respectively.

Replacing $f'(d(t))$ to the ratio between the time derivatives of the objective function and the decision variable, we have

$$\ddot{d}(t) = -a\dot{d}(t) - c\dot{f}(d(t))\Big/\dot{d}(t) \tag{7}$$

In the above equation, we can use the estimate $\hat{\dot{f}}(d(t))$ obtained by the adaptive velocity estimator instead of the time derivative, $\dot{f}(d(t))$. The proposed optimizer is given by

$$\ddot{d}(t)\dot{d}(t) + a\left(\dot{d}(t)\right)^2 = c\hat{\dot{f}}(d(t)) \tag{8}$$

The time derivative $\dot{d}(t)$ can be obtained by using a differential equation solver via Simulink as shown in Figure 1.

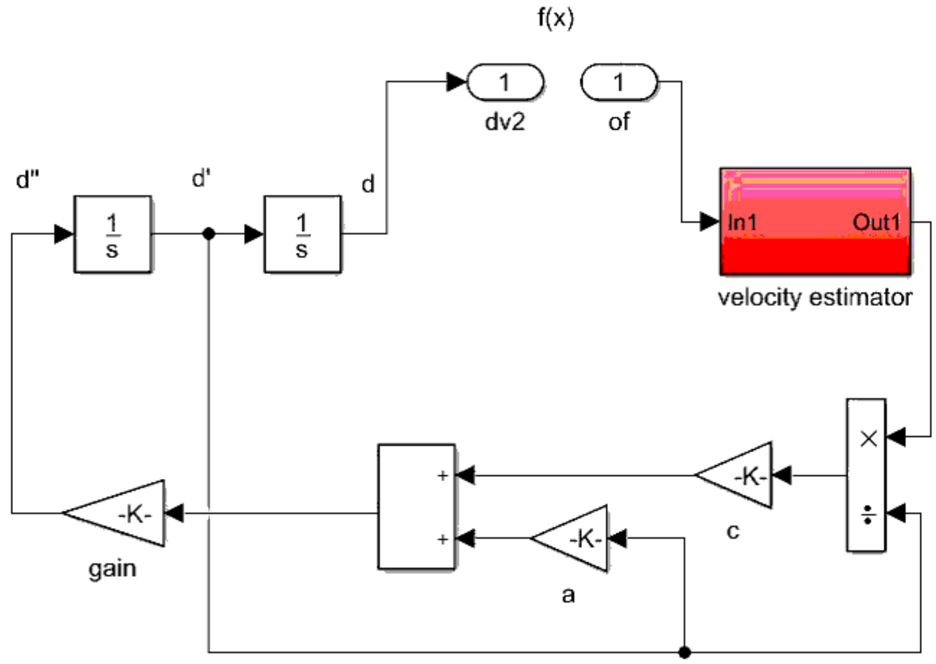

FIGURE 1. Momentum method with a single decision variable via Simulink

To extend to multivariable case, we propose the switching optimizer by using multiple single variable optimizers to obtain the partial derivatives of the objective function. The switching optimizer with two decision variables is given by

$$\begin{cases} \ddot{d}(t) = -a_1\dot{d}_1(t) - c_1\dot{f}(d_1(t)) \Big/ \dot{d}_1(t), & t \in [2n\Delta, (2n+1)\Delta) \\ \dot{d}_1(t) = 0, & t \in [(2n+1)\Delta, (2n+2)\Delta) \end{cases} \tag{9}$$

$$\begin{cases} \ddot{d}_2(t) = -a_2\dot{d}_2(t) - c_2\dot{f}(d_2(t)) \Big/ \dot{d}_2(t) & t \in [(2n+1)\Delta, (2n+2)\Delta) \\ \dot{d}_2(t) = 0, & t \in [2n\Delta, (2n+1)\Delta) \quad n = 0, 1, 2, \dots \end{cases} \tag{10}$$

where Δ is a design parameter that means a time interval to execute one optimizer and is tuned manually so that the objective function is smaller. The proposed optimizer updates each decision variable independently for each time interval.

2.4. **Numerical examples.** The parameters of the adaptive velocity estimator are selected as $k = 10$ and $\gamma_1 = 30$. We consider the following time-varying parabolic function in two variables:

$$f(x_1, x_2, t) = 10\left(x_1 - \frac{1}{t+1}\right)^2 + (x_2 - 1)^2 \tag{11}$$

where t denotes a time variable. We can search the minimum value of the parabolic function by using the measurement $f(x_1, x_2, t)$ for each time step. In this example, we can apply the switching optimizer by regarding the objective function as $f(x_1, x_2, t)$ and the decision variable as x_1, x_2. The switching optimizer can be implemented in Simulink shown in Figure 2, where switching is achieved by using a rectangular pulse function with a period of 1 [sec], an amplitude of 1, and a duty ratio of 50%. The period of the pulse function is tuned manually so that the objective function is smaller. Other parameters of the pulse function are fixed values.

Figure 3 shows the convergence processes of the objective function and the decision variables. The parameters and the initial values are selected as indicated in Table 1. The swithing optimizer converges to the minimum value of the objective function.

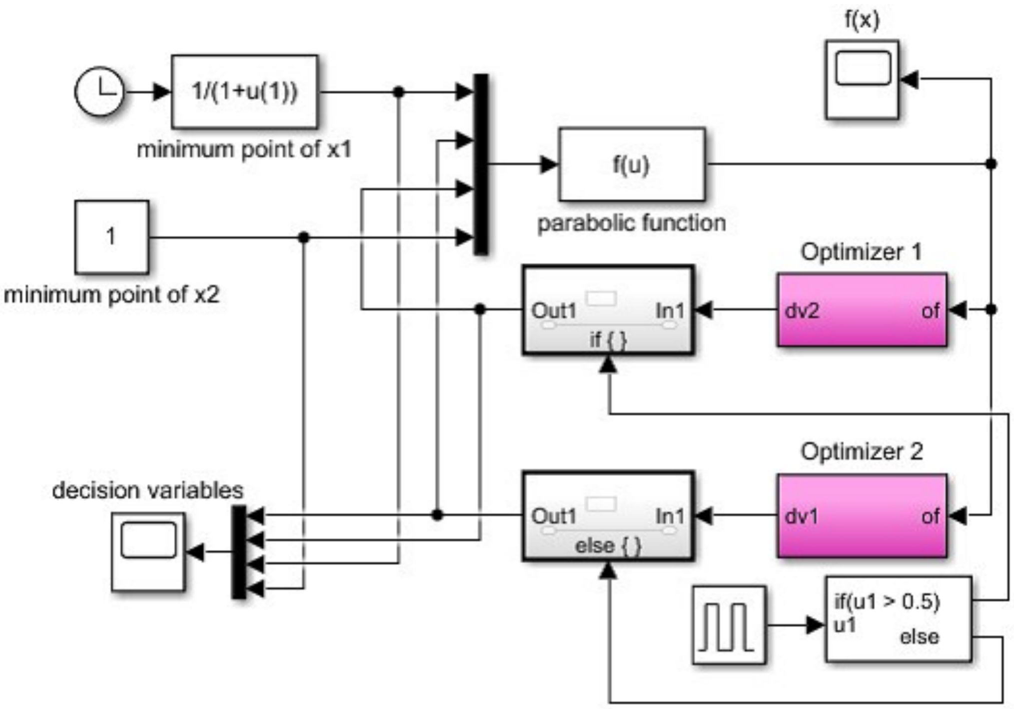

FIGURE 2. Switching optimizer for two decision variables via Simulink

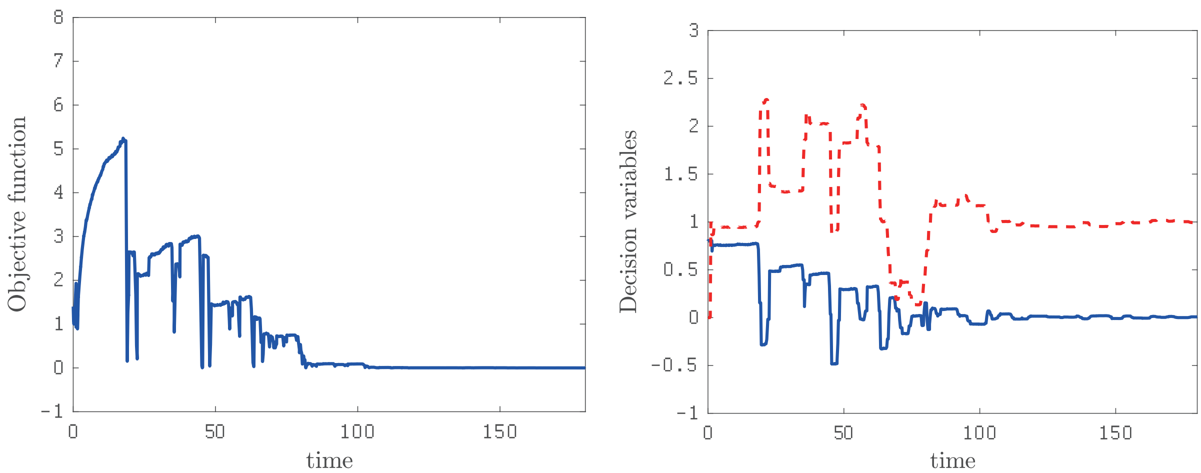

FIGURE 3. Convergence processes of the objective function and the decision variables each time step: (left) the objective function $f(x_1, x_2, t)$, and (right) decision variables

TABLE 1. Parameters in the switching optimizer

Variables	Optimizer 1	Optimizer 2
a_1, a_2	1500	1500
c_1, c_2	750	500
$x_1(0)$, $x_2(0)$	0.8	0
$x_1'(0)$, $x_2'(0)$	12	12

3. **Signal Separation of CAM.** The proposed switching optimizer is applied to the signal separetion problem of CAM.

3.1. **Minimal CAM model.** The CAM model that we used has been previously studied by Blasius et al. (see [4, 5]) and herein, we only outline the minimal CAM model. The model can be characterized by the major reactant pools of CAM that generate the carbon flow during the circadian cycle. The pool concentrations are as follows:

- internal CO_2 concentration, w;
- malate concentration in the cytoplasm, x;
- malate concentration in the vacuole, y; and
- z denotes a variable that describes the ordering of the lipid molecules in the tonoplast membrane.

These are the dynamic variables of the cyclic process, which are connected by the flows, u_1, u_2, and u_3, during the gain and loss terms of the metabolites. The model depends on three external control parameters: temperature, T, light intensity, L, and external CO_2 concentration, C_{ext}. The CAM model of a single cell can be rewritten in the state-space form as follows:

$$\left.\begin{array}{l} \dot{\tilde{x}} = \tilde{f}\,(\tilde{x}, L, T) + \tilde{g}_1(w)(C_{ext}(t) - w) + \tilde{g}_2 L(t) \\ \tilde{x} = \begin{bmatrix} w \\ x \\ y \\ z \end{bmatrix}, \quad \tilde{f} = \begin{bmatrix} \dfrac{1}{\epsilon}(-u_2 + R_{co2}) \\ \dfrac{1}{\epsilon}(-u_1 + u_2) \\ u_1 \\ \dfrac{1}{\tau}(g(z,T) - y) \end{bmatrix} \\ \tilde{g}_1 = \begin{bmatrix} \dfrac{1}{\epsilon}\dfrac{c_J}{\exp(\alpha w)} \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \tilde{g}_2 = \begin{bmatrix} \dfrac{w}{\epsilon} \\ 0 \\ 0 \\ 0 \end{bmatrix} \end{array}\right\} \tag{12}$$

$$\left.\begin{array}{l} u_1 = cx - \dfrac{y}{z} \\ u_2 = \dfrac{w}{x} - x \\ u_3 = J_{co2} - C_{co2} + R_{co2} \\ J_{co2} = c_J \dfrac{(C_{ext}(t) - w)}{\exp(\alpha w)} \\ C_{co2} = L(t) w \\ R_{co2} = c_R \dfrac{L_K}{L(t) + L_K} \dfrac{w_1}{w + w_1} \end{array}\right\} \tag{13}$$

where the variables and the parameters are defined as follows:

w, x, y, and z: states variables
T: temperature, control parameter
L: light intensity, control parameter
C_{ext}: external CO_2 concentration, control parameter
ϵ: time constant
τ: time constant
c, c_J, c_R, L_K, w_1, α: constants
$g(z,T)$: thermodynamic equilibrium value of malate concentration in the vacuole
u_1: the difference between malate influx and efflux into and out of the vacuole, modeled with the dynamic hysteresis

u_2: the difference between malate production from CO_2 fixation by phosphoenolpyruvate carboxylase (PEPc) and its depletion by decarboxylation

u_3: the difference between CO_2 influx and efflux

J_{co2}: CO_2 uptake from outside

C_{co2}: CO_2 consumption by photosynthesis, which is directly proportional to the external control parameter light intensity, $L(t)$

R_{co2}: CO_2 production by respiration

Blasius et al. calculated the dynamic behavior by using the dimensionless variables with parameters [4]: $C_{ext} = 1$, $L(t) = 1$, $T = 0.2238, 0.2242, 0.2246, 0.2250, 0.2254$, $c = 5.5$, $c_J = 1$, $c_R = 1$, $\varepsilon = 0.001$, $\tau = 0.35$, $\alpha = 1.5$, $w_1 = 0.1$, $L_K = 0.5$, and $R = 0.1$. The nonlinear function $g(z, T)$ is shown in [4].

3.2. **Signal separation.** The biological clock is a spatiotemporal product of many weakly coupled individual oscillators, defined by the metabolic constraints of CAM [11]. Takahashi et al. showed that the shoot apex is composed of an ensemble of coupled clocks that influence rhythms in roots [12]. We make the following assumptions about CAM dynamics.

1) CO_2 uptake for each cell is proportional to cell volume.
2) Cells are connected by vascular bundle to export photosynthetic products. Delays in cell dynamics result from these transport delays.

We express the whole CO_2 uptake model as

$$J_{co2}^{all}(t) = \sum_k \alpha_k J_{co2}^k(t - L_k) \tag{14}$$

where J_{co2}^k denotes the CO_2 uptake of the kth cell, J_{co2}^{all} denotes the whole CO_2 uptake of a CAM plant, k denotes a cell number, and α_k and L_k denote the volume and the transfer delay of the kth cell. Knowing the delay times of the signals, L_k's, can often help to understand the physiology of a plant, e.g., the delay time can indicate a transport delay of a starch via a vascular bundle. Further, the model is useful to control the biological rhythm of the plant. We define an identification problem of the delay sequence of the CO_2 uptake as follows:

Estimate the parameters L_k's and α_k's so as to minimize the objective function $f(t)$:

$$f(t) = \left(J_{co2}^{all}(t) - \hat{J}_{co2}^{all}(t)\right)^2 \tag{15}$$

where $J_{co2}^{all}(t)$ denotes measurement signal by CO_2 analyzer and $\hat{J}_{co2}^{all}(t)$ is calculated using the equation:

$$\hat{J}_{co2}^{all}(t) = \sum_k \hat{\alpha}_k J_{co2}^k\left(t - \hat{L}_k\right) \tag{16}$$

The plant cell has many different parts. In the simulation, we consider the representative cells for two parts such as a blade, and petiole. The parameters are $\alpha_1 = 1$, $\alpha_2 = 0.8$, $L_1 = 0$, $L_2 = 1$. It is supposed that α_1, L_1 are known, we estimate α_2, L_2 so as to minimize the objective function $f(t)$. The decision variable is selected as

$$d = \begin{bmatrix} \hat{\alpha}_2 & \hat{L}_2 \end{bmatrix} \tag{17}$$

The switching optimizer is applied to finding a minimum of the objective function (15) where $k = 2$. The parameters and the initial values are selected as $a_1 = a_2 = 1500$, $c_1 = c_2 = 2500$, $\hat{\alpha}_2(0) = 0.7$, $\dot{\hat{\alpha}}_2(0) = 15$, $\hat{L}_2(0) = 0.6$, $\dot{\hat{L}}_2(0) = 15$. The switching of the optimizer is achieved by using the rectangular pulse function with a period of 0.2, an amplitude of 1, and a duty ratio of 50%. The period of the pulse function must be adjusted manually according to the situation of convergence of an objective function. The

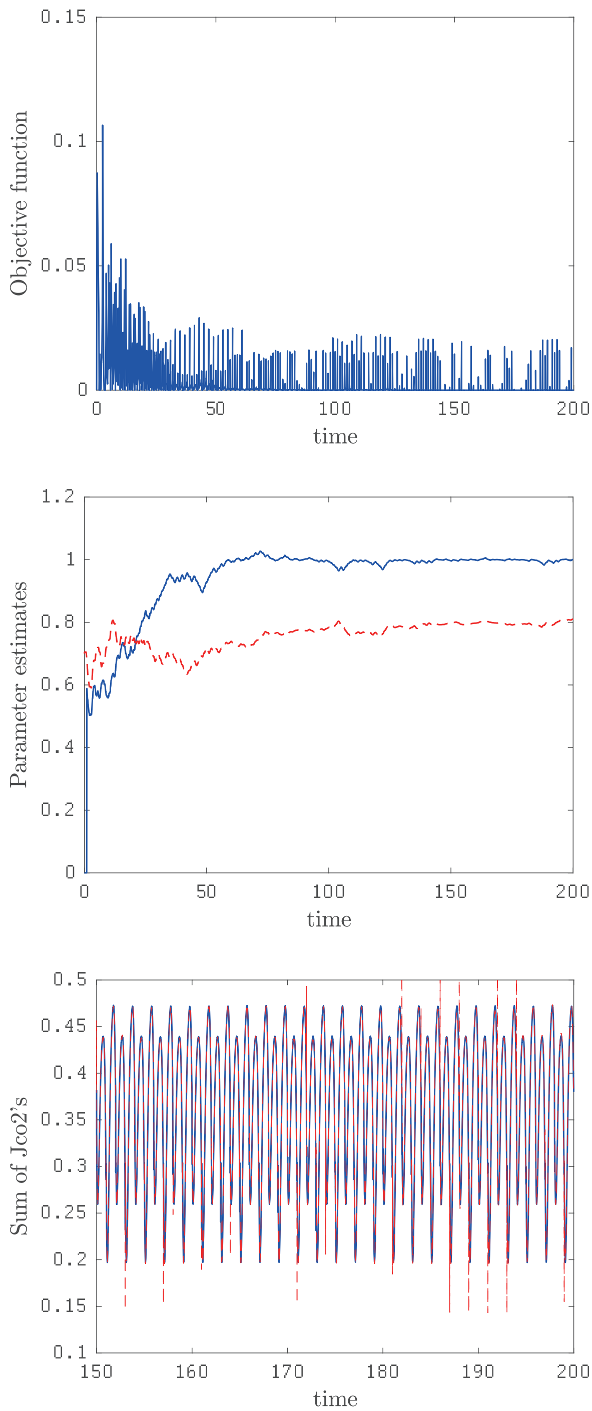

FIGURE 4. Time evolution of the proposed real-time optimizer where all axes are dimensionless: (top) objective function $P(t)$, (middle) decision variables $\hat{\alpha}_2$ (dotted red line) and $\hat{L}_2$ (solid blue line), and (bottom) J_{co2}^{all} (solid blue line) and $\hat{J}_{co2}^{all}(t)$ (dotted red line)

amplitude and the duty ration are fixed values. Figure 4 shows the objective function, the decision variables, and the estimate of the whole CO_2 uptake. As the objective function becomes small, the estimation error of the whole CO_2 uptake, $\left|J_{co2}^{all}(t) - \hat{J}_{co2}^{all}(t)\right|$ is also small as shown in Figure 4. The estimates $\hat{\alpha}_2$ and $\hat{L}_2$ stay near their true values after enough time has passed. The identification errors of the parameters, $|\alpha_2 - \hat{\alpha}_2|$ and $\left|L_2 - \hat{L}_2\right|$, become small.

4. **Conclusion.** In this paper, we presented a model of the sum of the CO_2 uptake of CAM plants as a linear combination of delayed oscillation waves of cells. Further, we proposed a continuous-time momentum gradient descent for searching for a minimum of the objective function and apply this optimization method to the signal separation problem. The proposed switching optimizer is effective for multivariable real-time optimization problems. The estimated parameters tell us the cell-cell interactions. We just assembled the experimental equipment by using an incubator and try to collect CO_2 uptake data. The next problem we would consider is to apply the proposed method to experimental data.

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