APPLICATION OF SPSA TECHNIQUES IN NONLINEAR SYSTEM IDENTIFICATION

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Abstract

Simultaneous perturbation stochastic approximation (SPSA) is an optimization method which requires only a few objective function evaluations to obtain gradient information. In this paper, a first-order SPSA algorithm is described, which makes use of several numerical artifices, including adaptive gain sequences, gradient smoothing and a step rejection procedure, to enhance convergence and stability. This algorithm is particularly well suited to problems involving a large number of parameters and its potentialities are demonstrated in the context of nonlinear system identification. First, a relatively simple example is considered, i.e. the development of a neural network state space model for a level-control system. Second, a more advanced application is studied, i.e. the estimation of the most-likely kinetic parameters and initial conditions of a bioprocess model describing the evolution of a few macroscopic components in batch animal cell cultures.

1 Introduction

Over the past several years, nonlinear models have been increasingly used for simulation, state estimation and control purposes. Particularly, the rapid progresses in computational techniques and the success of nonlinear model predictive control have been strong incentives for the development of such models as neural networks or first-principle models.

Process modeling requires the estimation of several unknown parameters from noisy measurement data. A least-squares or maximum likelihood cost function (depending on the assumptions on the measurement noise) is usually minimized using a gradient-based optimization method.

Several techniques for computing the gradient of the cost function are available, including finite difference approximations and analytic differentiation. This latter technique leads to backpropagation in neural networks (NN) or sensitivity equations in the case of conventional first-principle models.

In the above-mentioned techniques, the computational expense required to estimate the current gradient direction is directly proportional to the number of unknown model parameters, which becomes an issue for models involving a large number of parameters. This is typically the case in NN modeling, but can also occur in other circumstances, such as the estimation of parameters and initial conditions in first principle models. Moreover, the derivation of sensitivity equations requires analytic manipulation of the model equation, which is time consuming and subject to errors (note that an important stream of current research and developments is dedicated to the automatic generation of such equations using symbolic manipulation).

In contrast to standard finite differences which approximate the gradient by varying the parameters one at a time, the simultaneous perturbation (SP) approximation of the gradient proposed by Spall [6] makes use of a very efficient technique based on a simultaneous (random) perturbation in all the parameters. Hence, one gradient evaluation requires only two evaluations of the cost function. This approach has first been applied to gradient estimation in a first-order stochastic approximation (SA) algorithm [6], and more recently to Hessian estimation in an accelerated second-order SPSA algorithm [7].

In previous works [4, 9], the authors have applied the above-mentioned first- and second-order SA algorithms (1SPSA and 2SPSA) to weights and biases estimation in NNs. Efficiency, simplicity of implementation and very modest computational costs make 1SPSA particularly attractive, even though it suffers from the classical drawback of first-order algorithms, i.e., a slowing down in the convergence as an optimum is approached (note that this phenomenon is even more pronounced in the case of SP techniques since the gradient information is more delicate to "extract" in the – usually rather "flat" - neighborhood of the optimum).

In this study, a variation of the original first-order algorithm is considered which makes use of adaptive gain sequences, gradient smoothing and a step rejection procedure, to enhance convergence and stability. To demonstrate the algorithm efficiency and versatility, attention is focused on two application examples:

1. the estimation of the weights and biases of a neural state space model for a level-control system (i.e., the classical one tank problem, which is investigated in simulation here);
2. the estimation of kinetic parameters (and initial conditions) of a macroscopic model of animal cell cultures by minimizing a maximum-likelihood criterion based on the experimental measurements of biomass, glucose, glutamine and lactate concentrations.

This paper is organized as follows. Section 2 introduces the basic principle of the first-order SPSA algorithm used throughout this study. In section 3, the algorithm is applied to NN modeling of a level-control system. At this stage, attention is paid to the careful selection of input signals and to the NN parameter estimation procedure. Section 4 deals with a more advanced application, namely the maximum likelihood estimation of kinetic parameters and initial conditions of a bioprocess model from experimental measurements of several macroscopic component concentrations. Direct and cross-validation results demonstrate the good model agreement. Finally, section 5 is devoted to some concluding remarks.

2 A first-order SPSA algorithm

Consider the problem of minimizing a, possibly noisy, objective function $J(\theta)$ with respect to a vector θ of unknown parameters

1SPSA is given by the following core recursion for the parameter vector θ [6]

$$\hat{\theta}_k = \hat{\theta}_{k-1} - a_k \, \hat{g}_k(\hat{\theta}_{k-1}) \qquad (1)$$

in which a_k is a non-negative scalar gain coefficient, and $\hat{g}_k(\hat{\theta}_{k-1})$ is an approximation of the criterion gradient obtained by varying all the elements of $\hat{\theta}_{k-1}$ simultaneously, i.e.,

$$\hat{g}(\theta_{k-1}) = \begin{bmatrix} \dfrac{J(\hat{\theta}_{k-1} + c_k\Delta_k) - J(\hat{\theta}_{k-1} - c_k\Delta_k)}{2c_k\Delta_{k1}} \\ \cdots \\ \dfrac{J(\hat{\theta}_{k-1} + c_k\Delta_k) - J(\hat{\theta}_{k-1} - c_k\Delta_k)}{2c_k\Delta_{kp}} \end{bmatrix} \qquad (2)$$

where c_k is a positive scalar and $\Delta_k = (\Delta_{k1}, \Delta_{k2}, \ldots, \Delta_{kp})^T$ with symmetrically Bernouilli distributed random variables $\{\Delta_{ki}\}$.

In its original formulation, 1SPSA makes use of decaying gain sequences $\{a_k\}$ and $\{c_k\}$ in the form

$$a_k = \frac{a}{(A+k+1)^\alpha}, \qquad c_k = \frac{c}{(k+1)^\gamma} \qquad (3)$$

Numerical experiments show that the algorithm may therefore get stuck somewhere in the parameter space if the criterion value becomes significantly worse (due to a poor current gradient approximation, a non-convex optimization problem,...) and the gain sequences are too small to recover from this situation.

In order to enhance convergence and stability, the use of an adaptive gain sequence for parameter updating is considered in this study, i.e.,

$$\begin{aligned} a_k &= \eta\, a_{k-1}, \quad \eta \geq 1, \quad \text{if } J(\theta_k) < (1+\beta)J(\theta_{k-1}) \\ a_k &= \mu\, a_{k-1}, \quad \mu \leq 1, \quad \text{if } J(\theta_k) \geq (1+\beta)J(\theta_{k-1}) \end{aligned} \qquad (4)$$

In addition to gain attenuation when the value of the criterion becomes worse, "blocking" mechanisms [7] are also applied, i.e., the current step is rejected and, starting from the previous parameter estimate, a new step is accomplished (with a new gradient evaluation and a reduced updating gain). The parameter β in (4) represents the permissible increase in the criterion, before step rejection and gain attenuation occur.

A constant gain sequence $c_k = c$ could be used for gradient approximation, the value of c being selected so as to overcome the influence of (numerical or experimental) noise. In the optimum neighborhood, a decaying sequence in the form (3) is required to evaluate the gradient with enough accuracy and avoid an amplification of the "slowing down" effect mentioned in the previous section.

Finally, a gradient smoothing (GS) procedure is implemented, i.e., gradient approximations are averaged across iterations in the following way

$$G_k = \rho_k\, G_{k-1} + (1-\rho_k)\,\hat{g}_k(\hat{\theta}_{k-1}), \quad 0 \leq \rho_k \leq 1, \quad G_0 = 0 \qquad (5)$$

where, starting with an initial value of $\rho = \rho_0$, ρ_k is decreased in a way similar to (4) when step rejection occurs (i.e. $\rho_k = \mu\rho_{k-1}$ with $\mu \leq 1$) and is reset to its initial value after a successful step.

The use of these numerical artifices, i.e., adaptive gain sequences, step rejection procedure and gradient smoothing, significantly improves the effective practical performance of the algorithm (which, in the following, is denoted "adaptive 1SP-GS").

Inequality constraints can also be taken into account by a projection algorithm introduced in [5] (the current parameter estimate is projected onto a closed set included in the admissible region in such a way that no function evaluation is required outside this latter region). In this study, bound constraints (e.g., positivity constraints) are handled in this way.

3 NN modeling of a level control system

Consider a cylindrical tank which is operated with inlet and outlet flow rates $Q_{in}(t)$ and $Q_{out}(t)$, respectively. $Q_{out}(t)$ results from the liquid free flow through the outlet valve and can be computed using a Toricelli law in the form

$$Q_{out}(t) = \alpha S_v(t)\sqrt{2gh(t)} \qquad (6)$$

where h(t) is the liquid level in the tank, g is the gravity acceleration, $S_v(t)$ is the surface area of the valve (whose aperture will be kept constant in the following) and α is a correction factor.

The inlet flow rate $Q_{in}(t)$ can be manipulated (via a pump) to control the liquid level in the tank, which is simply given by

$$S_t \frac{dh}{dt} = Q_{in}(t) - Q_{out}(t) \qquad (7)$$

where S_t is the cross section area of the tank.

Equations (6-7) define the process which is investigated in simulation in the rest of this section. Our objective is to develop a NN model describing the dynamic evolution of the tank level h(t) in response to changes in the inlet flow rate $Q_{in}(t)$.

When modeling nonlinear dynamic systems, several alternative NN architectures can be used (see, e.g. [3]). Here, a neural state space model [8] is selected

$$\begin{aligned} \hat{x}_{k+1} &= W_{AB} \tanh(V_A \hat{x}_k + V_B u_k + \beta_{AB}) \\ \hat{y}_k &= W_{CD} \tanh(V_C \hat{x}_k + V_D u_k + \beta_{CD}) \end{aligned} \qquad (8)$$

As illustrated in Fig. 1, neural state space models are recurrent NNs. The dimensions of the weight matrices and bias vectors are $W_{AB} \in \Re^{n \times n_{hx}}$, $V_A \in \Re^{n_{hx} \times n}$, $V_B \in \Re^{n_{hx} \times m}$, $\beta_{AB} \in \Re^{n_{hx}}$, $W_{CD} \in \Re^{\ell \times n_{hy}}$, $V_C \in \Re^{n_{hy} \times n}$, $V_D \in \Re^{n_{hy} \times m}$, $\beta_{CD} \in \Re^{n_{hy}}$, where n = 1, m = 1, ℓ = 1, n_{hx} = 5 and n_{hy} = 2 are the selected number of states, inputs, outputs and hidden neurons, respectively.

The 28 unknown parameters are estimated from a set of N system outputs y_i (at times t_i, i=1,...,N) by minimizing a least-square criterion, i.e.

$$\min_{\theta} J_{ls}(\theta) = \min_{\theta} \sum_{i=1}^{N} (y_i - \hat{y}_i(\theta))^2 \qquad (9)$$

where $\hat{y}(\theta)$ is the NN prediction.

In this application example, a particular choice for the training data set is made, which consists of the system response to three input step sequences with decreasing step duration, i.e., ΔT_1 = 1000s, ΔT_2 = 300s and ΔT_3 = 100s. The idea here is to first use the data set with a relatively low frequency content and to minimize the least-square criterion (9) in order to obtain first parameter estimates. Then, starting from these first estimates, the criterion (9) is minimized using the data corresponding to the first two sequences. Finally, the procedure is repeated with the complete data set. This multistep training procedure appears to be particularly useful to alleviate the problem of local minima. The system response to the three input step sequences is compared to the prediction of the NN model in Fig. 2, which demonstrates the very good model agreement.

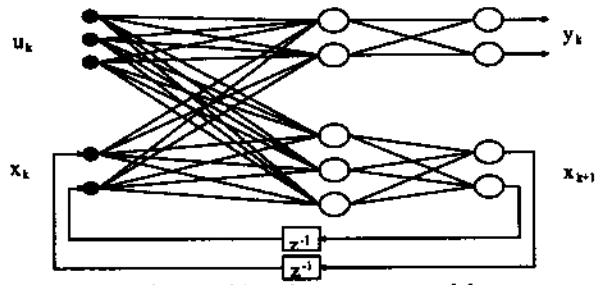

Figure 1: Neural state space model

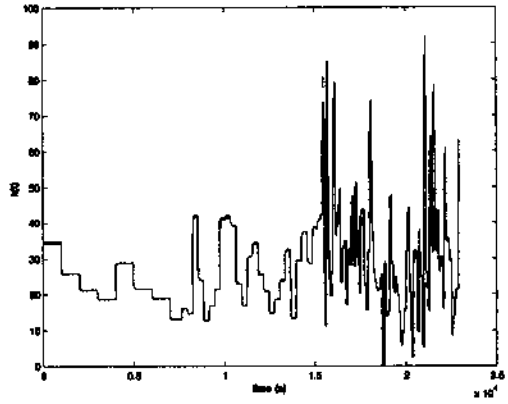

Figure 2: Comparison of the system response (solid line) to three input step sequences with decreasing step duration and the NN model prediction (dashed line)

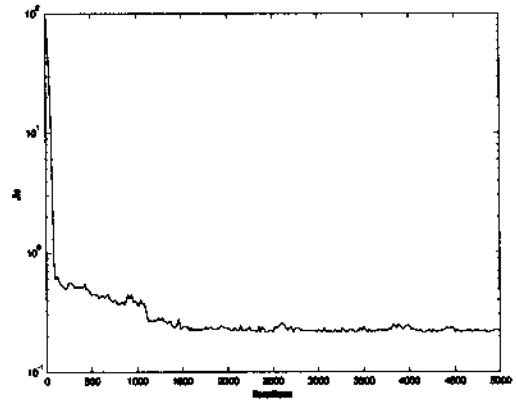

Figure 3: Convergence of the 1SP-GS algorithm (evolution of the criterion value as a function of the number of iterations) in the first training step

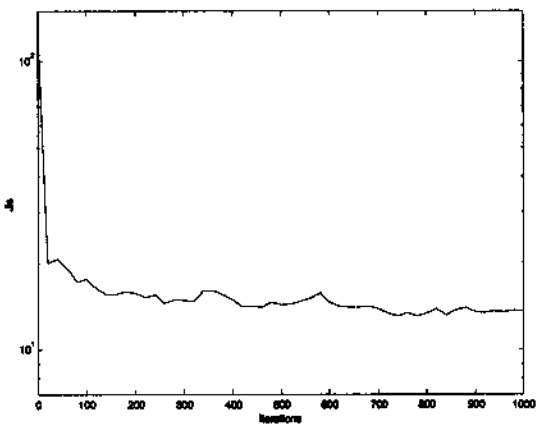

Figure 4: Convergence of the 1SP-GS in the third training step

The tuning parameters of the adaptive 1SP-GS algorithm are as follows: $c = 10^{-8}$, $\gamma = 1$ (a decaying sequence c_k in the form (3) is used to evaluate the criterion gradient), $a_0 = 10^{-5}$, $\eta = 1.05$, $\mu = 0.85$, $\beta = 0.02$ (a relative increase of 2% in the criterion is allowed), $\rho_0 = 0.75$. The convergence of the algorithm in the first training step (based on the first input sequence) is shown in figure 3 for the a total number of iterations $N = 5000$. The convergence of the algorithm in the third step (based on the complete data set) is shown in figure 4 for $N = 1000$ iterations. The slowing-down effect as an optimum is approached is clearly apparent.

4 Macrospic modeling of animal cell cultures

Consider batch animal cell cultures described by a simple macroscopic reaction scheme

growth: $$\nu_{G\,ln}\, G\,ln \xrightarrow{\varphi_g} \hat{} X \qquad (10)$$

maintenance: $$G + \nu_X X \xrightarrow{\varphi_m} \nu_X X + \nu_L L \qquad (11)$$

where X, G, Gln and L represent biomass, glucose, glutamine and lactate, respectively, and $\nu_{G\,ln}$, ν_X and ν_L are pseudo-stoechiometric coefficients. The symbol "$\rightarrow\hat{}$" means that the growth reaction is auto-catalyzed by X and the presence of "ν_X X" in both sides of the maintenance reaction means that X catalyzes this latter reaction.

The growth rate φ_g and the maintenance rate φ_m are described by a general kinetic model structure proposed in [2]

$$\varphi_g(X,G,G\,ln) = \alpha_g X^{\gamma_{g,X}} G\,ln^{\gamma_{g,Gln}} e^{-\beta_{g,G} G} \qquad (12)$$

$$\varphi_m(X,G) = \alpha_m X^{\gamma_{m,X}} G^{\gamma_{m,G}} e^{-\beta_{m,X} X} \qquad (13)$$

Simple mass balances allow the following dynamic model to be derived :

$$\frac{dX}{dt} = \varphi_g(X,G,G\,ln) \qquad X(0) = X_0 \qquad (14)$$

$$\frac{dG}{dt} = -\varphi_m(X,G) \qquad G(0) = G_0 \qquad (15)$$

$$\frac{dG\,ln}{dt} = -\nu_{G\,ln}\varphi_g(X,G,G\,ln) \qquad Gln(0) = Gln_0 \qquad (16)$$

$$\frac{dL}{dt} = \nu_L \varphi_m(X,G) \qquad L(0) = L_0 \qquad (17)$$

where X(t), G(t), Gln(t) and L(t) denote the respective component concentrations.

Identification of bioprocess models is a delicate task and in [2], a systematic procedure is proposed, which allows the pseudo-stoechiometric coefficients to be estimated independently of the kinetic coefficients [1] by minimizing a maximum likelihood criterion. This procedure also considers the estimation of the most likely initial conditions (since the concentration measurements are corrupted by noise at each sampling time, including the initial one).

In this study, we assume that the pseudo-stoechiometric coefficients have already been estimated following the above-mentioned procedure and that only the kinetic coefficients and the initial component concentrations have to be inferred from rare and asynchronous measurements of biomass, glucose, glutamine and lactate concentrations.

The measurement equation is given by

$$y(t_i) = x(t_i) + \varepsilon(t_i) \qquad i = 1,\ldots,N \qquad (18)$$

where $x(t_i) = [X(t_i)\ G(t_i)\ Gln(t_i)\ L(t_i)]^T$, $y(t_i)$ and $\varepsilon(t_i)$ are the state, measurement and noise vectors at time t_i, respectively. The measurement errors are assumed to be normally distributed, white noises with zero mean and variance matrix $Q(t_i)$.

Data are collected from seven batch experiments corresponding to different initial glucose and glutamine concentrations. Five of these experiments are used for parameter estimation, the two remaining ones being used for cross-validation tests.

The 28 unknown parameters (8 kinetic coefficients and 20 initial concentrations) are estimated by minimizing a maximum likelihood cost function taking into account the measurement noises, i.e.,

$$\min_{\theta} J_{ml}(\theta) = \min_{\theta} \frac{1}{2}\sum_{i=1}^{N} (y_i - \hat{x}_i(\theta))^T Q_i^{-1} (y_i - \hat{x}_i(\theta)) \qquad (19)$$

where y_i, Q_i and $\hat{x}_i(\theta)$ are the measurement vector, the measurement error covariance matrix and the state estimate obtained by integration of the model equations (12-17) with the parameters θ at time t_i, respectively.

The tuning parameters of the adaptive 1SP-GS algorithm are selected as follows: $c = 10^{-6}$, $\gamma = 1.5$ (a decaying sequence c_k

is used for gradient evaluation), $a_0 = 10^{-8}$, $\eta = 1.01$, $\mu = 0.$ = 0 (no relative increase in the criterion is allowed), $\rho_0 = ($ Starting with the measured initial concentrations (which affected by measurement errors) and an initial guess for kinetic parameters corresponding to a criterion value J 65760, the minimization (19) leads to a criterion value J 308 in 50000 iterations. This number of iterations m appear quite large at first sight, but the computational co very modest as each iteration only requires two crite evaluations (each of these evaluations involves 5 m simulations corresponding to the 5 experimental batches in this identification phase). On the other hand, stan centered finite difference approximations would require criterion evaluations per iteration !

The parameter estimates are listed in Table 1. Figu compares the measurement data of one of the experiments used in the parameter identification proce with the model prediction (direct validation), whereas Fi 5 shows the same kind of comparison with the measurer data of one of the remaining two experiments (cross-validation). In these graphs, the circled points are the measured data and the bars represent the 99% confidence intervals. The solid lines are the concentration trajectories predicted by the identified model.

These figures demonstrates the excellent model agreement

$\alpha_g = 0.0892$	$\alpha_m = 0.0341$
$\gamma_{g,X} = 0.4609$	$\gamma_{m,X} = 1.1395$
$\gamma_{g,G\,ln} = 0.1728$	$\gamma_{m,G} = 0.0822$
$\beta_{g,G} = 0.0089$	$\beta_{m,X} = 0.0980$

Table 1: Parameter estimates

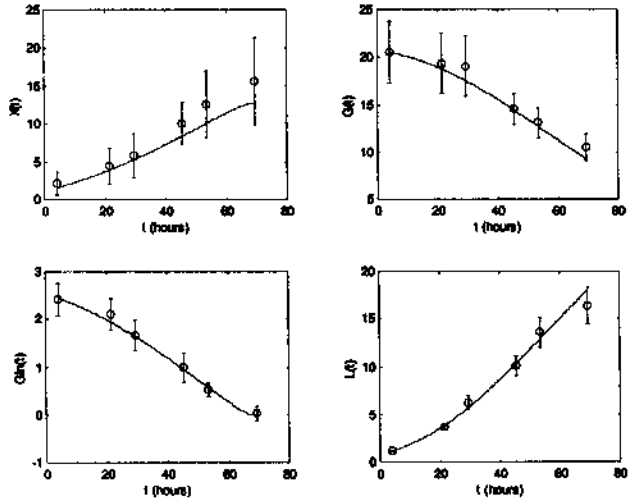

Figure 4: Direct validation

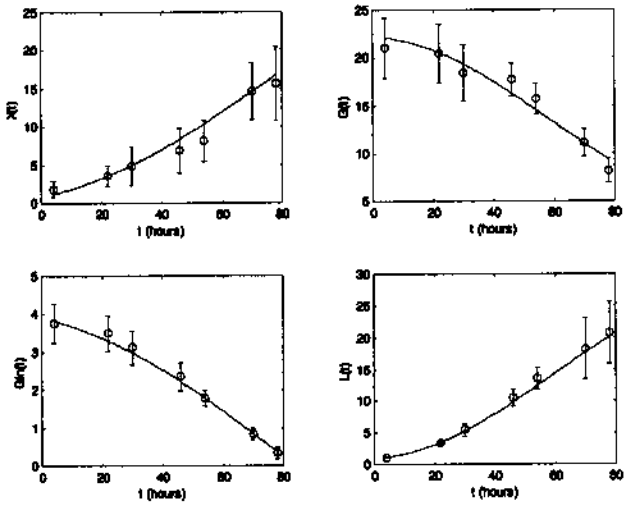

Figure 5: Cross-validation

5 Conclusion

The simultaneous perturbation approach developed by Spall [6, 7] is a very powerful technique, which allows an approximation of the gradient of the objective function to be computed by effecting simultaneous random perturbations in all the parameters. Therefore, this approach is particularly well-suited to problems involving a relatively large number of design parameters. In this study, a first-order SP algorithm is described and applied to application examples in nonlinear system identification. First, the weights and biases of a neural network modeling a level control system is accomplished by minimizing an output error least-square criterion. Second, a maximum-likelihood approach is used to estimate the kinetic parameters and the initial condition of a bioprocess model from experimental measurements of a few macroscopic components. These applications, as well as previous authors studies [4, 9], demonstrate the usefulness of the proposed SP-algorithm.

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