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Comparison of Gradient Estimation Methods for Real-time Optimization

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Abstract

Various real-time optimization techniques proceed by controlling the gradient to zero. These methods primarily differ in the way the gradient is estimated. This paper compares various gradient estimation methods. It is argued that methods with model-based gradient estimation converge faster but can be inaccurate in the presence of plant-model mismatch. In contrast, model-free methods are accurate but typically take longer to converge.

Keywords: Real-time optimization, Extremum-seeking control, Neighboring extremals, Self-optimizing control, Gradient estimation.

1. Introduction

Process optimization based on first-principles models is challenging due to the complexity of the underlying physico-chemical processes. Hence, simpler models are typically formulated and used for optimization by updating their parameters on-line using measurements. Alternatively, measurements can also be used to update the inputs without the intermediary of a physical model.

Any measurement-based optimization approach will (i) select the active constraints and keep them active, and (ii) push the reduced gradients to zero. To do so, one needs to measure or estimate the constraints, the gradients of the constraints, and the gradient of the cost function. Constraints are often straightforward to measure. In contrast, gradients must be estimated since they cannot be measured directly.

This paper explores various ways of estimating gradients in real time for optimizing the steady-state performance of dynamic processes. In particular, gradient estimation techniques are classified as either model-based or model-free, and each class is analyzed in terms of accuracy and convergence time.

2. Real-time Optimization using Gradient Control

2.1. Problem formulation

In this paper, the *unconstrained* optimization of a process at steady state is considered, which can be formulated as follows:

$$\min_u J \quad = \quad \phi(x,u,\theta) \qquad \text{s.t.} \quad \dot{x} = F(x,u,\theta) \equiv 0, \tag{1}$$

where J is the cost to be minimized, $x \in \Re^n$ the states (considered at equilibrium), $u \in \Re^m$ the inputs, and $\theta \in \Re^q$ the uncertain parameters. In addition, it is assumed that

$y = h(x,u,\theta)$, where $y \in \Re^p$ are the measurements. F, h, and ϕ are smooth functions that describe the system dynamics, the outputs, and the cost function, respectively. It is assumed that the state variables can be expressed as functions of u and θ by using (1) and thus can be eliminated to give the following optimization problem:

$$\min_u J \quad = \quad \Phi(u,\theta) \qquad y = H(u,\theta), \tag{2}$$

where Φ and H are corresponding lumped functions. Let θ_0 be the nominal parameter values, u_0 the nominal optimal inputs and y_0 the nominal optimal outputs.

The necessary conditions of optimality indicate that the derivative $g = \frac{\partial J}{\partial u} = 0$. All the real-time optimization methods presented in this work will adapt the input to force the gradient to zero. They only differ in the way the gradient is computed. With k being the adaptation gain in $[\mathrm{h}^{-1}]$ and P an approximation of the Hessian, the general adaptation law is $\dot{u}_{opt} = -kP^{-1}g$.

2.2. Model-free gradient estimation techniques

In all the model-free techniques, it is assumed that the cost is directly measured, i.e. $y = J$. Also, since no structural information regarding F is available, the gradient can only be obtained by presenting the system with different input values and calculating the gradient from the corresponding output values. The presentation is for the single-input case, but it can be easily extended to the multi-input scenario.

Finite-difference gradient estimation (FD) - Kreysig (1988): Two different input values are given over a period of time T, which allows the system to each time reach steady state. The gradient is computed using the finite difference, with i the iteration number:

$$u(t) = \begin{cases} u_{opt}(i) & 2iT \le t < (2i+1)T \\ u_{opt}(i)+\Delta & (2i+1)T \le t < (2i+2)T \end{cases}, g = \frac{J((2i+2)T) - J((2i+1)T)}{\Delta}. \tag{3}$$

Gradient estimation by excitation/correlation (EC) - Ariyur and Krstic (2003): A sinusoidal excitation is added and the gradient estimated by correlation:

$$u(t) = u_{opt}(t) + \Delta\sin(\omega t), \quad \frac{d\bar{J}}{dt} = \alpha(J-\bar{J}), \quad \frac{dg}{dt} = \beta\left(\frac{2(J-\bar{J})\sin(\omega t)}{\Delta} - g\right), \tag{4}$$

where α and β represent filter coefficients. The first filter eliminates the bias and the second determines the gradient. The frequency of excitation is so chosen that the period of oscillation is slower than the system settling time.

Gradient estimation from multiple units (MU) - Srinivasan (2007): The availability of multiple process units is assumed, and the inputs to the units differ by an offset. The gradient is estimated using finite difference between units (labeled 'a' and 'b' here):

$$u_a(t) = u_{opt}(t) + \frac{\Delta}{2}, \quad u_b(t) = u_{opt}(t) - \frac{\Delta}{2}, \quad g(t) = \frac{J_a(t) - J_b(t)}{\Delta}. \tag{5}$$

2.3 Model-based gradient estimation techniques

In model-based techniques, it is assumed that a structurally correct process model is available. However, the parameters θ are either unknown or uncertain. Furthermore, it will be assumed that there are more measurements than the number of uncertain parameters, i.e.

$p \geq q$. Since the measured information is sufficient to estimate the unknown parameters, there will be no external excitation, and $u(t) = u_{opt}(t)$.

Parameter estimation - gradient calculation (PE) - Adetola and Guay (2007): This is the classical two-step method, whereby the parameters are estimated and the updated model used for calculating the gradient. Numerical optimization is replaced by controlling the gradient to zero. With $\hat{\theta}$ the parameter estimate and k_θ the gain used in parameter estimation, one has:

$$\dot{\hat{\theta}} = k_\theta \left(\frac{\partial H}{\partial \theta}\right)^+ (y - H(u,\hat{\theta})), \quad \hat{\theta}(0) = \theta_0, \qquad g = \frac{\partial \Phi}{\partial u}(\hat{\theta}). \tag{6}$$

Neighboring extremals (NE) - Gros et al. (2009): The parametric variation $\delta\theta = \theta - \theta_0$ is calculated from the variations $\delta u = u - u_0$ and $\delta y = y - y_0$, respectively:

$$\delta y = \frac{\partial H}{\partial \theta}\delta\theta + \frac{\partial H}{\partial u}\delta u \qquad \rightarrow \qquad \delta\theta = \left(\frac{\partial H}{\partial \theta}\right)^+ (\delta y - \frac{\partial H}{\partial u}\delta u). \tag{7}$$

Then, from variational calculations, the gradient is given by:

$$g = \frac{\partial^2 \Phi}{\partial u^2}\delta u + \frac{\partial^2 \Phi}{\partial u \partial \theta}\delta\theta = \frac{\partial^2 \Phi}{\partial u \partial \theta}\left(\frac{\partial H}{\partial \theta}\right)^+ \delta y + \left(\frac{\partial^2 \Phi}{\partial u^2} - \frac{\partial^2 \Phi}{\partial u \partial \theta}\left(\frac{\partial H}{\partial \theta}\right)^+ \frac{\partial H}{\partial u}\right)\delta u. \tag{8}$$

Self-optimizing control (SOC) - Alstad and Skogestad (2007): This method calculates the sensitivity of the optimal outputs and inputs with respect to parametric variations. From the variational form of the necessary conditions (8), the sensitivity matrix becomes:

$$S = \begin{bmatrix} \frac{\partial y_{opt}}{\partial \theta} \\ \frac{\partial u_{opt}}{\partial \theta} \end{bmatrix} = \begin{bmatrix} \frac{\partial H}{\partial \theta} - \frac{\partial H}{\partial u}\left(\frac{\partial^2 \Phi}{\partial u^2}\right)^{-1}\frac{\partial^2 \Phi}{\partial u \partial \theta} \\ -\left(\frac{\partial^2 \Phi}{\partial u^2}\right)^{-1}\frac{\partial^2 \Phi}{\partial u \partial \theta} \end{bmatrix}, \; g = N \begin{bmatrix} \delta y \\ \delta u \end{bmatrix}, \; P = N \begin{bmatrix} \frac{\partial y_{opt}}{\partial u} \\ I_m \end{bmatrix}, \tag{9}$$

where the $m \times (p+m)$ matrix N lies in the null space of S^T and I_m is the $m \times m$ identity matrix. The m controlled variables are selected as $c = N\,[\delta y, \delta u]^T$, which indeed represents the gradient.

3. Comparison of Gradient Estimation Techniques

The goal of this section is to compare the various gradient estimation techniques in terms of their basic requirements as well as accuracy and convergence characteristics.

Measurements: Model-free methods require only the cost to be measured, whereas model-based methods rely on output measurements. Note that the model relates the measured outputs y to the cost J, thereby making cost measurement unnecessary.

Model: Among the various model-based techniques, only PE uses the model on-line, while the other two use the model off-line to design the controller.

Excitation: In model-based techniques, since information regarding uncertainty can be obtained from the outputs, no temporal excitation is necessary. In contrast, in model-free techniques with only cost measurement, one needs to excite the system to estimate the gradient. Temporal excitation is provided in the FD and EC methods, while the use of multiple units provides the needed excitation in the MU method.

Accuracy: Model-based techniques work well when the model is structurally correct and the disturbances can be represented by parametric variations. When there is plant-model mismatch or when there are other variations that are not accounted for, the convergence will not be to the desired optimum. Since NE and SOC are based on linearization, they tend to give good results only for small parametric variations.

Convergence time: Model-based techniques have a clear edge when it comes to convergence time. Except for the MU adaptation, model-free methods are slow since the excitation has to respect a certain time-scale separation and be slower than the system settling time. MU adaptation is faster since the excitation is not temporal. Among the model-based techniques, PE is slower due to the dynamics of the parameter adaptation. In NE and SOC, the gradient information is readily available, which makes them fast.

4. Illustrative Example

Steady-state optimization of an isothermal CSTR is investigated, with the reactions $A + B \rightarrow C$, $2B \rightarrow D$. The manipulated variables are the feed rates of A and B. The following cost function is considered:

$$\max_{u_A,u_B} \quad J = \frac{c_C^2 (u_A + u_B)^2}{u_A c_{A\,in}} - w(u_A^2 + u_B^2). \tag{10}$$

The first term of J corresponds to the product of the amount of C produced $c_C (u_A + u_B)$ and the yield factor $\frac{c_C(u_A+u_B)}{u_A c_{A\,in}}$, while the second term penalizes the control effort with $w = 0.004$. The model equations result from standard mass balances and read:

$$\dot{c_A} = -k_1\, c_A\, c_B + \frac{u_A}{V} c_{A\,in} - \frac{u_A + u_B}{V} c_A = 0, \qquad \dot{c_C} = k_1\, c_A\, c_B - \frac{u_A + u_B}{V} c_C = 0, \tag{11}$$

$$\dot{c_B} = -k_1\, c_A\, c_B - 2\, k_2\, c_B^2 + \frac{u_B}{V} c_{B\,in} - \frac{u_A + u_B}{V} c_B = 0, \quad \dot{c_D} = k_2\, c_B^2 - \frac{u_A + u_B}{V} c_D = 0. \tag{12}$$

where c_X denote the concentration of species X, $V = 500$ L the reactor volume, $c_{A\,in} = 2$ mol/L and $c_{B\,in} = 1.5$ mol/L the inlet concentrations and $k_1 = 0.75$ L/(mol h) and $k_2 = 1.5$ L/(mol h) the rate constants of the two chemical reactions. The parameters that are subject to change are $\theta = [k_1\ k_2]^T$, with the plant values being $k_{1\,plant} = 1.4$ L/(mol h) and $k_{2\,plant} = 0.4$ L/(mol h). In addition, an unmodeled disturbance, $c_{A\,in,plant} = 2.5$ mol/L is considered to study the effect of plant-model mismatch.

The values of the adaptation gain k are given in Table 1. All methods use the Hessian evaluated at the nominal optimum for the matrix P, except for the SOC method that uses (9). All model-free methods use $\Delta = 0.4\,\mathrm{Lh}^{-1}$. The EC method uses $\omega_1 = 2\pi/150$, $\omega_2 = 2\pi/200$, $\alpha = \beta_1 = \beta_2 = 1/200\ \mathrm{h}^{-1}$. The parameter estimation uses $k_\theta = 1\ \mathrm{h}^{-1}$.

Table 1 also summarizes the results obtained with the different approaches, in terms of accuracy (optimality loss) and convergence time, with and without plant-model mismatch. The normalized cost is computed by dividing the actual plants cost $J(t)$ by the corresponding steady-state optimal cost J^*. Thus, the optimality loss is given upon convergence by $\eta = 1 - \frac{J(T_{conv})}{J^*}$, where T_{conv} is the convergence time. In addition, Figure 1 depicts the evolution of the normalized cost for the six methods for the case of plant-model mismatch. The model-based methods are clearly less accurate. However, these methods do quite well in the case of a perfect model, for which case the optimality loss is practically zero with the PE scheme, while small errors persist with NE and SOC due to the effect of

linearization. In terms of convergence time, PE is slightly inferior due to the time taken for parameter estimation. Model-free methods are able to reject the effect of both parametric uncertainty and plant-model mismatch at the price of a larger convergence time (thousands of hours for FD and EC and about 150 hours for MU).

		No model mismatch $c_{Ain,plant} = 2\,\frac{\text{mol}}{\text{l}}$		Model mismatch $c_{Ain,plant} = 2.5\,\frac{\text{mol}}{\text{l}}$	
Strategy	$k\,[h^{-1}]$	T_{conv} [h]	η [%]	T_{conv} [h]	η [%]
No adapt	-	-	19.06	-	26.35
FD	0.003	1200	0.22	1200	0.07
EC	0.001	3000	0.44	4000	0.33
MU	0.02	150	0.03	150	0.05
PE	0.1	75	0.001	75	6.82
NE	1	45	0.50	50	4.89
SOC	1	45	0.84	60	17.39

Table 1. Convergence time and optimal loss of model-free (FD, EC and MU) and model-based methods (PE, NE and SOC) for the cases without and with plant-model mismatch.

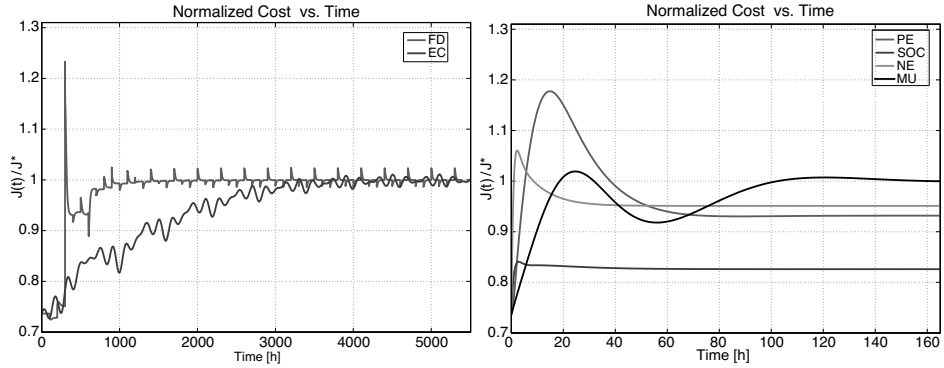

Figure 1. Normalized cost for the case of plant-model mismatch (model-free methods FD, EC and MU converge to the optimal cost, whereas model-based methods do not).

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