

Nonlinear Adaptive Control of a Chemical Reactor

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Abstract: – The paper deals with continuous-time nonlinear adaptive control of a continuous stirred tank reactor. The control strategy is based on an application of the controller consisting of a linear and nonlinear part. The static nonlinear part is derived in the way of an inversion and exponential approximation of measured or simulated input-output data. The design of the dynamic linear part is based on approximation of nonlinear elements in the control loop by a continuous-time external linear model with directly estimated parameters. In the control design procedure, the polynomial approach with the pole assignment method is used. The nonlinear adaptive control is tested by simulations on the nonlinear model of the CSTR with a consecutive exothermic reaction.

Key-Words: - Chemical reactor, nonlinear control, adaptive control, polynomial method, pole assignment. NC theory are described in e.g. [1], [8] or [15].

1 Introduction

From the system theory point of view, continuous stirred tank reactors (CSTRs) belong to a class of nonlinear systems with mathematical models described by sets of nonlinear differential equations. Various models of CSTRs can be found in e.g. [4], [10] and [12].

It is well known that the control of chemical reactors often represents very complex problem. The control problems are due to the process nonlinearity, high input-output sensitivity as well as to other unpleasant behaviour. The process with such properties is hardly controllable by conventional control methods, and, its effective control requires application some of advanced methods.

One possible method to cope with this problem exploits a linear adaptive controller with parameters computed and readjusted on the basis of recursively estimated parameters of an appropriate chosen continuous-time external linear model (CT ELM) of the process. Some results obtained by this method can be found in e.g. [5] and [6].

An effective approach to the control of CSTRs and similar processes utilizes various methods of the nonlinear control (NC). Several modifications of the

Especially, a part of the NC methods exploits factorization of nonlinear models of the plants on linear and nonlinear parts, e.g. [2], [3], [13], [14] or [16].

In this paper, the CSTR control strategy is based on an application of the controller consisting of a static nonlinear part (SNP) and dynamic linear part (DLP). The static nonlinear part is obtained from simulated or measured steady-state characteristic of the CSTR, its inversion, exponential approximation, and, subsequently, its differentiation. On behalf of development of the linear part, the SNP including the nonlinear model of the CSTR is approximated by a CT external linear model. For the CT ELM parameter estimation, the direct estimation in terms of filtered variables is used, see e.g. [7] and [11]. Then, the resulting CT controller is derived using the polynomial approach and pole assignment method, e.g. [9]. The simulations are performed on a nonlinear model of the CSTR with a consecutive exothermic reaction.

2 Model of the CSTR

Consider a CSTR with the first order consecutive

exothermic reaction according to the scheme $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ and with a perfectly mixed cooling jacket. Using the usual simplifications, the model of the CSTR is described by four nonlinear differential equations

$$\frac{dc_A}{dt} = -\left(\frac{q_r}{V_r} + k_1\right)c_A + \frac{q_r}{V_r}c_{Af} \quad (1)$$

$$\frac{dc_B}{dt} = -\left(\frac{q_r}{V_r} + k_2\right)c_B + k_1c_A + \frac{q_r}{V_r}c_{Bf} \quad (2)$$

$$\frac{dT_r}{dt} = \frac{h_r}{(\rho c_p)_r} + \frac{q_r}{V_r}(T_{rf} - T_r) + \frac{A_h U}{V_r(\rho c_p)_r}(T_c - T_r) \quad (3)$$

$$\frac{dT_c}{dt} = \frac{q_c}{V_c}(T_{cf} - T_c) + \frac{A_h U}{V_c(\rho c_p)_c}(T_r - T_c) \quad (4)$$

with initial conditions $c_A(0) = c_A^s$, $c_B(0) = c_B^s$, $T_r(0) = T_r^s$ and $T_c(0) = T_c^s$. Here, t is the time, c are concentrations, T are temperatures, V are volumes, ρ are densities, c_p are specific heat capacities, q are volumetric flow rates, A_h is the heat exchange surface area and U is the heat transfer coefficient. The subscripts are denoted $(\cdot)_r$ for the reactant mixture, $(\cdot)_c$ for the coolant, $(\cdot)_f$ for steady-state inputs and the superscript $(\cdot)^s$ for initial conditions. The reaction rates and the reaction heat are expressed as

$$k_j = k_{0j} \exp\left(\frac{-E_j}{RT_r}\right), j = 1, 2 \quad (5)$$

$$h_r = h_1 k_1 c_A + h_2 k_2 c_B \quad (6)$$

where k_0 are pre-exponential factors, E are activation energies and h are reaction enthalpies. The values of all parameters, inlet values and steady-state values with used units are given in Table 1.

Table 1. Parameters, steady-state inputs and initial conditions.

$V_r = 1.2 \text{ m}^3$	$c_{pr} = 4.05 \text{ kJ kg}^{-1}\text{K}^{-1}$
$V_c = 0.64 \text{ m}^3$	$c_{pc} = 4.18 \text{ kJ kg}^{-1}\text{K}^{-1}$
$\rho_r = 985 \text{ kg m}^{-3}$	$A_h = 5.5 \text{ m}^2$
$\rho_c = 998 \text{ kg m}^{-3}$	$U = 43.5 \text{ kJ m}^{-2}\text{min}^{-1}\text{K}^{-1}$
$k_{10} = 5.616 \times 10^{16} \text{ min}^{-1}$	$E_1/R = 13477 \text{ K}$
$k_{20} = 1.128 \times 10^{18} \text{ min}^{-1}$	$E_2/R = 15290 \text{ K}$
$h_1 = 4.8 \times 10^4 \text{ kJ kmol}^{-1}$	$h_2 = 2.2 \times 10^4 \text{ kJ kmol}^{-1}$
$c_A^s = 1.5796 \text{ kmol m}^{-3}$	$c_B^s = 1.1975 \text{ kmol m}^{-3}$
$T_r^s = 324.80 \text{ K}$	$T_c^s = 306.28 \text{ K}$
$c_{Af}^s = 2.85 \text{ kmol m}^{-3}$	$c_{Bf}^s = 0 \text{ kmol m}^{-3}$
$T_{rf}^s = 323 \text{ K}$	$T_{cf}^s = 293 \text{ K}$
$q_r^s = 0.08 \text{ m}^3\text{min}^{-1}$	$q_c^s = 0.08 \text{ m}^3\text{min}^{-1}$

In term of the practice, only the coolant flow rate can be taken into account as the control input. As the controlled output, the reactant temperature is considered. For the control purposes, the control input $u(t)$ and the controlled output $y(t)$ are defined as deviations from steady values

$$u(t) = q_c(t) - q_c^s, \quad y(t) = T_r(t) - T_r^s \quad (7)$$

The dependence of the reactant temperature on the coolant flow rate in the steady-state is in Fig. 1.

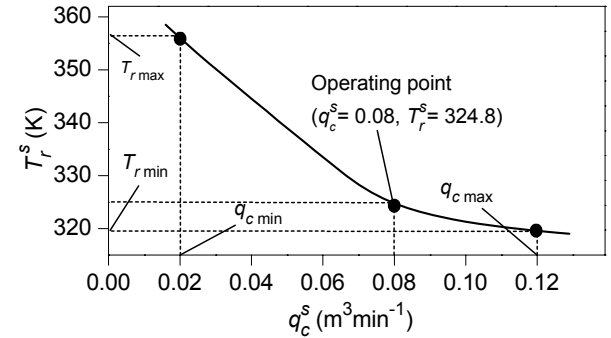


Fig. 1. Dependence of the reactant temperature on the coolant flow rate in the steady-state.

In subsequent control simulations, the operating interval for q_c has been determined as

$$q_{c \min} \leq q_c(t) \leq q_{c \max} \quad (8)$$

With regard to the purposes of a latter steady-state characteristic approximation, the values q_{cL} and q_{cU} are established that denote the lower and upper bound of q_c^s used for the approximation, and, T_{rU} and T_{rL} to them corresponding temperatures.

3 Controller Design

As previously introduced, the controller consist of a static nonlinear part and a dynamic linear part as shown in Fig. 2.

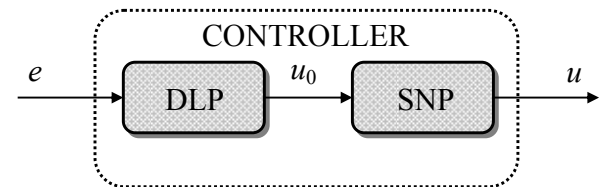


Fig. 2. The controller scheme.

The DLP creates a linear dynamic relation between the tracking error $e(t)$ and $u_0(t) = \Delta T_{rw}(t)$ which represents a difference of the reactant temperature adequate to its desired value. Then, the SNP generates a static nonlinear relation between u_0 and a

corresponding increment (decrement) of the coolant flow rate.

3.1 Nonlinear part of the controller

The SNP derivation appears from a simulated or measured steady-state characteristic. The coordinates on the graph axis are defined as

$$\gamma = \frac{q_c^s - q_{cL}}{q_{cL}}, \quad \psi = T_r^s - T_{rL} \quad (9)$$

where q_{cL} is the lower bound in the interval

$$q_{cL} \leq q_c^s \leq q_{cU} \quad (10)$$

and, T_{rL} is the temperature corresponding to q_{cU} .

It can be recommended to select the interval (10) slightly longer than (8). In this paper, lower and upper values in (8) and (10) were chosen $q_{cL} = 0.016$, $q_{c\min} = 0.02$, $q_{c\max} = 0.12$, and $q_{cU} = 0.13$.

In term of the practice, it can be supposed that the measured data will be affected by measurement errors. The simulated steady-state characteristic that corresponds to reality is shown in Fig. 3.

Making the replacement of coordinates, the inverse of this characteristic can be approximated by a function from the ring of polynomial, exponential, rational, eventually, by

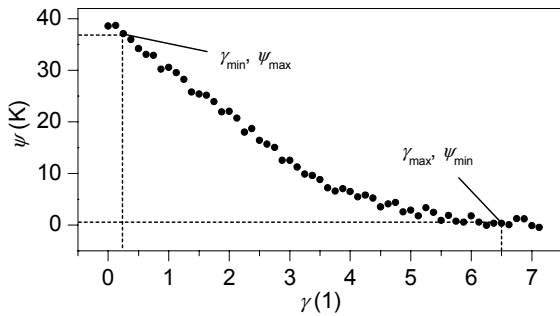


Fig. 3. Simulated characteristics $\psi = f(\gamma)$.

other type functions. Here, the second order exponential approximate function has been found in the form

$$\gamma = -74071.7 + 2.4589 \exp\left(-\frac{\psi}{3.967}\right) + 74076 \exp\left(-\frac{\psi}{697475}\right) \quad (11)$$

The inverse characteristic together with its approximation is in Fig. 4.

Now, a difference of the coolant flow rate $u(t) = \Delta q_c(t)$ in the output of the SNP can be

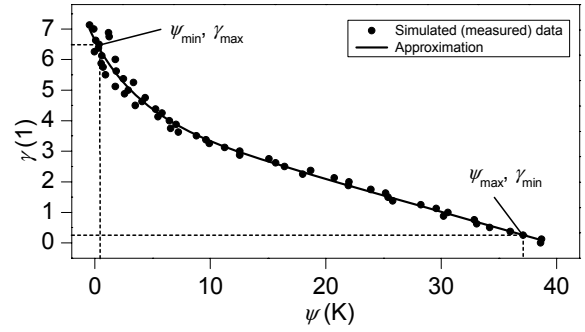


Fig. 4. Simulated and approximated inverse relation $\gamma = \varphi(\psi)$.

computed for each T_r as

$$u(t) = \Delta q_c(t) = q_{cL} \left(\frac{d\gamma}{d\psi} \right)_{\psi(T_r)} u_0(t) \quad (12)$$

The derivative of the approximate function (11) shown in Fig. 5 takes the form

$$\frac{d\gamma}{d\psi} = -0.6198 \exp\left(-\frac{\psi}{3.967}\right) - 0.1062 \exp\left(-\frac{\psi}{697475}\right)$$

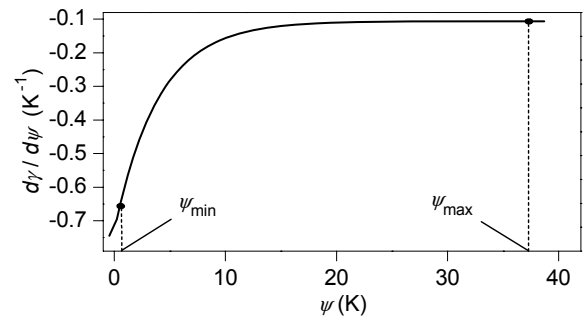


Fig. 5. Derivative of γ with respect to ψ .

3.2 CT external linear model of nonlinear elements

The second order CT ELM of the SNP in conjunction with a nonlinear model of the CSTR was chosen on the basis of pre-computed step responses of the SNP+CSTR in the form of the second order linear differential equation

$$\ddot{y}(t) + a_1 \dot{y}(t) + a_0 y(t) = b_0 u_0(t) \quad (13)$$

or, in the transfer function representation as

$$G(s) = \frac{Y(s)}{U_0(s)} = \frac{b(s)}{a(s)} = \frac{b_0}{s^2 + a_1 s + a_0} \quad (14)$$

where s is the complex variable (parameter of the Laplace transform).

3.3 CT ELM parameter estimation

The method of the CT ELM parameter estimation can be briefly carried out as follows.

Since the derivatives of both input and output cannot be directly measured, filtered variables u_{0f} and y_f are established as the outputs of filters

$$c(\sigma)u_{0f}(t) = u_0(t) \quad (15)$$

$$c(\sigma)y_f(t) = y(t) \quad (16)$$

where $\sigma = d/dt$ is the derivative operator, $c(\sigma)$ is a stable polynomial in σ that fulfills the condition $\deg c(\sigma) \geq \deg a(\sigma)$. It can be easily proved that the transfer behavior among filtered and among nonfiltered variables are equivalent. Using the L -transform of (15) and (16), the expressions

$$c(s)U_{0f}(s) = U_0(s) + \mu_1(s) \quad (17)$$

$$c(s)Y_f(s) = Y(s) + \mu_2(s) \quad (18)$$

can be obtained with μ_1 and μ_2 as polynomials of initial conditions. Substituting (17) and (18) into (14), and, after some manipulations, the relation between transforms of the filtered input and output takes the form

$$\begin{aligned} Y_f(s) &= \frac{b(s)}{a(s)}U_{0f}(s) + M(s) = \\ &= G(s)U_{0f}(s) + M(s) \end{aligned} \quad (19)$$

where $M(s)$ is a rational function as the transform of any function $\mu(t)$ which expresses an influence of initial conditions of filtered variables.

The filtered variables including their derivatives can be sampled from filters (15) and (16) in discrete time intervals $t_k = k T_s$, $k = 0, 1, 2, \dots$ where T_s is the sampling period. Denoting $\deg a = n$ and $\deg b = m$, the regression vector is defined as

$$\Phi(t_k) = \begin{bmatrix} -y_f(t_k) - y_f^{(1)}(t_k) \dots - y_f^{(n-1)}(t_k) \\ u_{0f}(t_k) u_{0f}^{(1)}(t_k) \dots u_{0f}^{(m)}(t_k) \ 1 \end{bmatrix}. \quad (20)$$

Now, the vector of parameters

$$\Theta^T(t_k) = [a_0 \ a_1 \ \dots \ a_{n-1} \ b_0 \ b_1 \ \dots \ b_m] \quad (21)$$

can be estimated from the equation

$$y_f^{(n)}(t_k) = \Theta^T(t_k) \Phi(t_k) + \mu(t_k). \quad (22)$$

3.4 Linear part of the controller

The DLP is inserted into the control loop as shown in Fig. 6. In the scheme, w is the reference signal, v is the disturbance, y is the controlled output, u_0 is the input to the ELM and e is the tracking error.

The transfer function $G(s)$ of the ELM is given

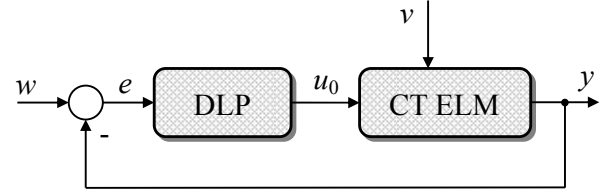


Fig. 6. Simplified scheme of the control loop.

by (14). Both the reference w and the disturbance v are considered to be step functions with transforms

$$W(s) = \frac{w_0}{s}, \quad V(s) = \frac{v_0}{s} \quad (23)$$

The transfer function of the DLP is in the form

$$Q(s) = \frac{U_0(s)}{E(s)} = \frac{q(s)}{p(s)} \quad (24)$$

where q and p are polynomials in s , and, $\deg q \leq \deg p$.

The controller design described in this section stems from the polynomial approach. General conditions required to govern the control system properties are formulated as stability, internal properness, asymptotic tracking of a step reference and step disturbance attenuation.

It is well known from the algebraic control theory that a controller which satisfies above requirements is in the polynomial ring given by a solution of the polynomial (Diophantine) equation

$$a(s)p(s) + b(s)q(s) = d(s) \quad (25)$$

with a stable polynomial $d(s)$ on the right side.

For step input signals w and v , the polynomial p is in the form

$$p(s) = s \tilde{p}(s). \quad (26)$$

For $\deg a = 2$ and step input signals, the degrees of unknown polynomials in (25) and (26) are given as

$$\deg q = 2, \quad \deg \tilde{p} = 1, \quad \deg d = 4 \quad (27)$$

and, the controller transfer function takes the form

$$Q(s) = \frac{q(s)}{s \tilde{p}(s)} = \frac{q_2 s^2 + q_1 s + q_0}{s(s + p_0)}. \quad (28)$$

In this paper, the polynomial d with roots determining the closed-loop poles is chosen as

$$d(s) = n(s)(s + \alpha)^2 \quad (29)$$

where n is a stable polynomial obtained by spectral factorization

$$a^*(s)a(s) = n^*(s)n(s) \quad (30)$$

and α is the selectable parameter that can usually be chosen by way of simulation experiments. Note that

a choice of d in the form (29) provides the control of a good quality for aperiodic controlled processes. The polynomial n has the form

$$n(s) = s^2 + n_1 s + n_0 \quad (31)$$

with coefficients

$$n_0 = \sqrt{a_0^2}, \quad n_1 = \sqrt{a_1^2 + 2n_0 - 2a_0}. \quad (32)$$

The controller parameters can be obtained from solution of the polynomial equation (25).

Evidently, the controller parameters can be adjusted by the selectable parameter α . The complete adaptive control system is shown in Fig. 7.

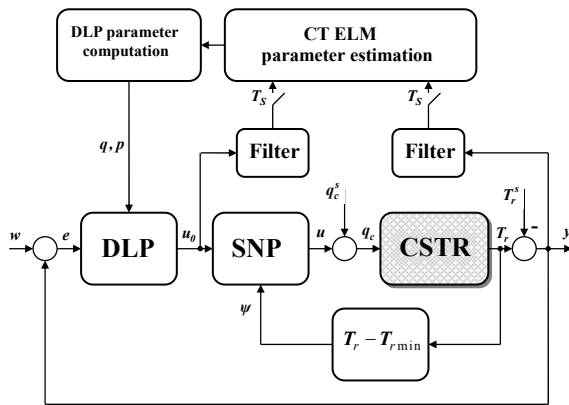


Fig. 7. Adaptive control system.

4 Control Simulations

The control simulations were performed in a neighbourhood of the operating point ($q_c^s = 0.08 \text{ m}^3 \text{ min}^{-1}$, $T_r^s = 324.8 \text{ K}$). For the start (the adaptation phase), a P controller with a small gain was used in all simulations.

The effect of the pole α on the control responses is transparent from Figs. 8 and 9. Here, on the basis of precomputed simulations, three values of α were selected. The control results show sensitivity of the controlled output and the input coolant flow rate to α . Obviously, careless selection of this parameter can lead to controlled outputs with overshoots or even to instability. Further, an increasing α leads to higher values and changes of the input signals. This fact can be important in control of some reactors where expressive input changes are undesirable.

A presence of the integrating part in the DLP enables rejection of various step disturbances entering into the process. Here, step disturbances $\Delta c_{Af} = \pm 0.1 \text{ kmol m}^{-3}$ at times $t_{v1} = 210 \text{ min}$ and $t_{v2} = 510 \text{ min}$ were injected into the CSTR. The DLP parameters were estimated only in the first

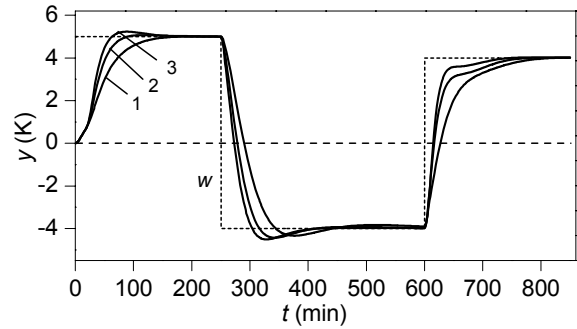


Fig. 8. Controlled output for $\alpha = 0.05$ (1), $\alpha = 0.075$ (2), $\alpha = 0.1$ (3).

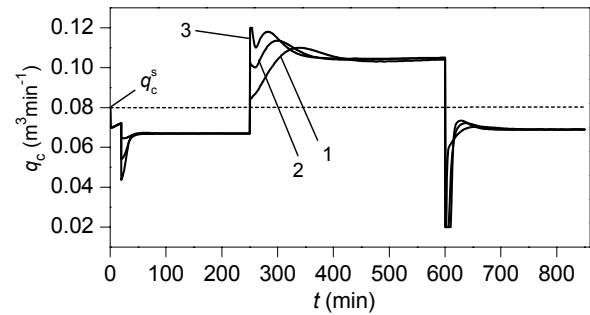


Fig. 9. Coolant flow rate for $\alpha = 0.05$ (1), $\alpha = 0.075$ (2), $\alpha = 0.1$ (3).

(tracking) interval $t < 200 \text{ min}$. The experiences of authors of this paper proved that an utilization of recursive identification in the phase of a constant reference and in a presence of step disturbances decreases the control quality. From this reason, during interval $t \geq 200 \text{ min}$, fixed DLP parameters were used. The controlled output responses are shown in Fig. 10.

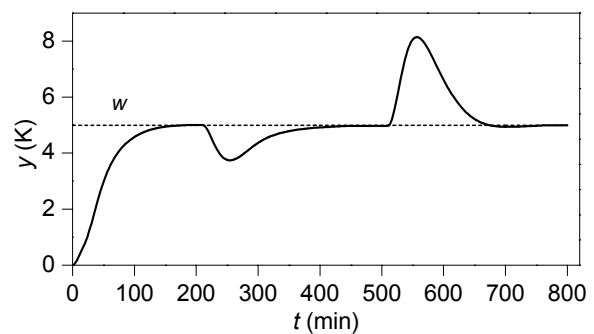


Fig. 10. Step disturbance rejection.

An influence of the SNP is evident from the control responses shown in Fig. 11. Here, the standard adaptive control without the nonlinear part of the controller was used. The simulation has been performed under the same conditions as by above presented cases for $\alpha = 0.075$. The responses in Fig. 11 show priority of the nonlinear control especially for greater changes of the reference signal.

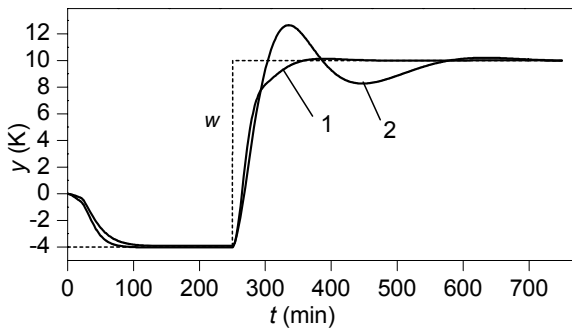


Fig. 11. Comparison of nonlinear adaptive control (1) with standard adaptive control (2).

5 Conclusions

In this paper, one approach to the nonlinear continuous-time adaptive control of the reactant temperature in a continuous stirred tank reactor was proposed. The control strategy is based on a factorization of a controller into the linear and the nonlinear part. A design of the controller nonlinear part employs simulated or measured steady-state characteristics of the process and their additional modifications. Then, the system consisting of the controller nonlinear part and a nonlinear model of the CSTR is approximated by a continuous time external linear model with parameters obtained through direct recursive parameter estimation. The resulting continuous-time controller linear part is derived using the polynomial approach and given by a solution of a polynomial equation. Tuning of its parameters is possible via closed-loop pole assignment. The presented method has been tested by computer simulation on the nonlinear model of the CSTR with a consecutive exothermic reaction. Simulation results demonstrated an applicability of the presented control strategy and its usefulness especially for greater changes of input signals in strongly nonlinear regions.

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