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Constrained Receding-Horizon Experiment Design and Parameter Estimation in the Presence of Poor Initial Conditions

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An optimal experiment design assumes the existence of an initial or nominal process model. The efficiency of this procedure depends on how the initial model is chosen. This creates a practical dilemma as estimating the model is precisely what the experiment tries to achieve. A novel approach to experiment design for identification of nonlinear systems is developed, with the purpose of reducing the influence of poor initial values. The experiment design and the parameter estimation are conducted iteratively under a receding-horizon framework. By taking steady-state prior knowledge into account, constraints on the parameters can be derived. Such constraints help reduce influence of poor initial models. The proposed algorithm is illustrated through examples to demonstrate its efficiency. © 2010 American Institute of Chemical Engineers *AIChE J,* 57: 2808–2820, 2011
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Introduction

Optimal experiment design aims at determining optimal experiment conditions to achieve a specific set of objectives. Experiment design is a broad subject that includes aspects such as input design, operating point design, and sampling time design. Although a significant amount of literature on optimal experiment design for linear systems has been published since the 1970s,[1,2] the optimal experiment design concerning nonlinear systems has remained largely unexplored.

One significant challenge for nonlinear experiment design as well as parameters identification is that the sensitivity functions used to search for optimal conditions depend on the unknown model parameters. Three existing methods have been proposed to address this challenge: minimax experiment design, ED (expectation of determinant)/EID (expectation of the inverse of determinant)-optimal design, and adaptive experiment design.

Minimax experiment design attempts to achieve robust experiment by minimizing the largest possible modeling error. This approach needs no prior information about parameter distributions. There are two recent representative publications on this topic. Rojas et al.[3] developed a method of optimizing the worst case of modeling error over the parameter set, while a convex optimization algorithm is implemented on a linear system. In conjunction, Welsh and Rojas[4] proposed an algorithm to solve a robust optimal experiment design problem by scenario approach. To construct convex or semidefinite convex problems, both techniques formulate the identification problem in frequency domain, but neither of the methods can be used for identification in nonlinear system. Moreover, the optimality objective function for nonlinear identification is generally difficult to be formulated as a convex or semidefinite convex problem.

Another group of methods (especially popular in bioscience fields) are experiment designs by optimizing over the expected determinant of a Fisher information matrix

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(FIM). Pronzato and Walter,[5] and Walter and Pronzato[6] proposed ED-optimal design and EID-optimal design as follows:

Definition 1 (Pronzato and Walter[5]). An experiment design φ_{ED} is called ED-optimal if

$$\varphi_{\mathrm{ED}} = \arg\min_{\varphi\in\Phi} E_{\hat{\theta}}[f(M(\hat{\theta},\varphi))] \quad (1)$$

Definition 2 (Walter and Pronzato[6]). An experiment design φ_{EID} is called EID-optimal if

$$\varphi_{\mathrm{EID}} = \arg\max_{\varphi\in\Phi} E_{\hat{\theta}}[1/f(M(\hat{\theta},\varphi))] \quad (2)$$

where φ is the experiment design, $\hat{\theta}$ is the estimate of parameter, E is the expectation operation, $M(\hat{\theta},\varphi)$ is the Fisher information matrix, and $f = \det(\cdot)^{-1}$.

Both of these two designs require prior knowledge of unknown parameter distributions.[7] Because in practice the prior parameter distributions and the expected value cannot be easily obtained, these methods can only apply to models with well-posed distributions.

Another solution is the adaptive design that is widely used in engineering literature.[8] The adaptive design starts from a nominal model guess $\hat{\theta}_0$, by which the design criterion $f(M(\hat{\theta}_0,\varphi))$ is optimized. Then, the experiment is conducted for the next one or several samples and the model parameter is identified. Afterward, the procedure iterates between experiment design and parameter estimation. In linear systems where unbiased or asymptotic unbiased estimation can be guaranteed, the adaptive design works well and eventually yields the optimal experimental condition for estimation. However, this method will likely fail in the case of nonlinear system identification under poor initial guess of the parameters. The poor initial guess problem is not uncommon especially when we have little prior knowledge about the true process in practice and is particularly harmful to the adaptive design. Poor initial conditions induce the problems in the following aspects:

The experiment design φ^* depends on the optimality criterion:

$$\varphi^* = \arg\min_{\varphi\in\Phi} f(M(\hat{\theta}_0,\varphi)) \quad (3)$$

Under an initial guess $\hat{\theta}_0$ that is far away from the real parameter, a design φ is far from the optimal or may even be very deviated from where a normal input signal should be; therefore, improper experiment conditions will be designed that may make the estimated parameter deviate further away from the optimal in subsequent iterations. This is particularly problematic for nonlinear systems.

Adaptive parameter estimation for nonlinear system cannot guarantee the convergence. In fact, the parameter estimator, typically an extended Kalman filter (EKF), is a local asymptotic observer only when some conditions being met such as the initial guess is near the true value or the system itself has weak nonlinearity.[9] Therefore, when the initial guess of the model parameters is poor, the parameter estimation through the EKF may diverge quickly.

Although there are numerous works on adaptive experiment design, to the best of authors' knowledge, none of them target solving poor initial condition problem. This problem is the principal concern of this work.

The remainder of this article is organized as follows: Section "Preliminaries" discusses preliminaries. In section "Receding-Horizon Experiment Design for Nonlinear System with Poor Initial Conditions", a new method is presented to solve the receding-horizon experiment design problem with poor initial conditions. To demonstrate the merits of the proposed method, two nonlinear examples are presented in section "Examples". The last section concludes the article.

Preliminaries

Sensitivity analysis

The sensitivity analysis method has been well developed over the last several decades[10]; in system identification, it is often used as a tool to assess estimability of parameters. Such estimability is described as the ability to compute parameters accurately given data and experimental conditions.[11,12] Increasing parameter sensitivity corresponds to better estimability. In optimal experiment design where we seek to obtain the most informative data, sensitivity analysis is particularly a valuable tool. Consider the system described by the following state space model

$$\dot{x}(t) = f(x(t), u(t), \theta) \quad (4)$$

$$y(t) = h(x(t), u(t), \theta) \quad (5)$$

where x is the state, f is state function of the state itself, input u and parameter θ, y is the output, and h is the output function. For illustrative purposes, we assume this system has p parameters, one state, one output, and $y(t) = x(t)$. The sensitivity is given by the following definition:

Definition 3 (Eslami[13]). Consider the system in (4) and (5). Assume that $\Delta\theta$ is the parameter variation for θ. Suppose that $y(t_k)$ changes to $y(t_k) + \Delta y(t_k)$ as $\theta \to \theta + \Delta\theta$, then the sensitivity (primitive-sensitivity) function of $y(t_k)$ in terms of θ is defined as the ratio of $\Delta y(t_k)/\Delta\theta$.

A sensitivity matrix can be computed as follows[11]

$$Z = \begin{bmatrix} \frac{\partial y}{\partial\theta_1}\big|_{t_1} & \frac{\partial y}{\partial\theta_2}\big|_{t_1} & \cdots & \frac{\partial y}{\partial\theta_p}\big|_{t_1} \\ \frac{\partial y}{\partial\theta_1}\big|_{t_2} & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ \frac{\partial y}{\partial\theta_1}\big|_{t_N} & \cdots & \cdots & \frac{\partial y}{\partial\theta_p}\big|_{t_N} \end{bmatrix} \quad (6)$$

where t_1 to t_N denote the start and end time of the experiment, respectively.

As an example, consider a model with parameter nonlinearity[12]

$$\dot{x}_t = -\frac{x_t}{\theta_1\theta_2} + \frac{u_t}{\theta_2} \quad (7)$$

$$y_t = x_t \quad (8)$$

The sensitivity matrix is calculated as[12]

$$\frac{\partial}{\partial\theta}\left(\frac{dx}{dt}\right) = \frac{\partial f}{\partial\theta} + \frac{\partial f}{\partial x}\frac{\partial x}{\partial\theta} \quad (9)$$

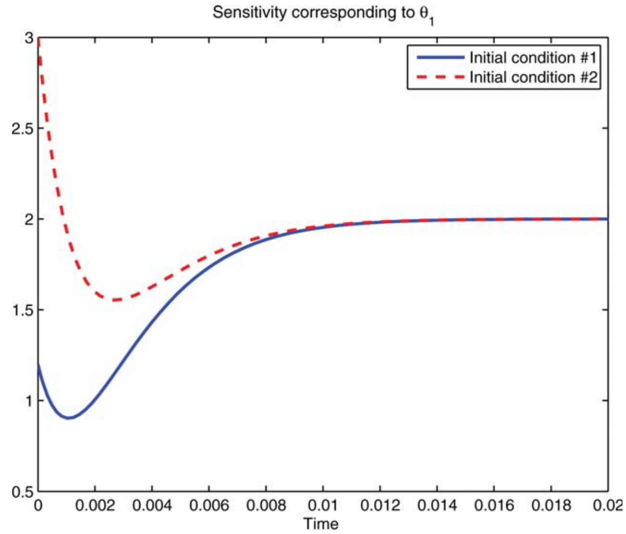

Figure 1. Sensitivities corresponding to different nominal values of parameters.

Blue solid line: initial values $E(\hat{\theta}_1^{(0)}) = 1.2, E(\hat{\theta}_2^{(0)}) = 0.0015$; red dash line: initial values $E(\hat{\theta}_1^{(0)}) = 3, E(\hat{\theta}_2^{(0)}) = 0.006$. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Rearrange Eq. 9

$$\frac{d}{dt}\left(\frac{\partial x}{\partial \theta}\right) = \frac{\partial f}{\partial \theta} + \frac{\partial f}{\partial x}\frac{\partial x}{\partial \theta} \tag{10}$$

Equation 10 is a differential equation from which the sensitivity ($\frac{\partial y}{\partial \theta} = \frac{\partial x}{\partial \theta}$ in this case) is calculated. Specifically

$$\frac{d}{dt}\left(\frac{\partial x}{\partial \theta_1}\right) = \frac{x}{\theta_1^2\theta_2} - \frac{1}{\theta_1\theta_2}\left(\frac{\partial x}{\partial \theta_1}\right) \tag{11}$$

$$\frac{d}{dt}\left(\frac{\partial x}{\partial \theta_2}\right) = \frac{x}{\theta_1\theta_2^2} - \frac{1}{\theta_1\theta_2}\left(\frac{\partial x}{\partial \theta_2}\right) - \frac{u}{\theta_2^2} \tag{12}$$

Equation 11 shows that when calculating the sensitivity matrix for models with parameters nonlinearity, parameters themselves are needed and so is the input. For illustrative purposes, Figure 1 shows that different nominal values of $\theta^{(0)}$ can lead to quite different sensitivities with respect to some parameters (θ_1 in this case), which may induce significant problems within the experiment design.

Information matrix

From Eq. 3, we know that the optimality criterion depends on the FIM. A commonly used optimality criterion is

$$f(M(\hat{\theta}_0, \varphi)) = -\log(\det(M(\hat{\theta}_0, \varphi))) \tag{13}$$

whose property has been discussed by Goodwin and Payne.[1] The relation between the sensitivity matrix and the FIM M is[11]

$$M = Z^T \Sigma^{-1} Z \tag{14}$$

where Z is sensitivity matrix defined in Eq. 6, and Σ is the covariance matrix of output y. In the case of covariance scaled response, Eq. 14 can be reduced to

$$M = Z^T Z \tag{15}$$

The advantage of the determinant criterion is its independence of the scaling of the parameters. This optimality criterion also minimizes the generalized covariance of the parameters estimate. The Cramér-Rao inequality is given by

$$P \equiv \mathrm{Cov}(\hat{\theta}) \geq M^{-1} \tag{16}$$

This inequality states that the inverse of the FIM acts as a lower bound for covariance of parameter estimate. When equality is satisfied, the estimator is said to be efficient.

For a class of unbiased estimators, the minimum variance estimator is statistically efficient. For nonlinear models, unbiased estimation has been widely known to be theoretically unapproachable. Song and Grizzle[9] showed that EKF, as a classical nonlinear approximation filter, can be an asymptotic unbiased estimator, although certain conditions such as a proper initial guess or a weak nonlinearity is required to achieve convergence. Practically, EKF works well in most nonlinear models.[14] In this work, we follow the principle that ‘‘maximizing the FIM corresponds to minimizing covariance of estimates,’’ as stated in most of the experiment design methodologies. Therefore, the optimality criterion in Eq. 13 is used for minimizing the covariance of $\hat{\theta}$.

Receding-Horizon Experiment Design for Nonlinear System with Poor Initial Conditions

Because of the impact of poor initial conditions on nonlinear system identification, it is desirable to derive a method that is robust both in experiment design and parameter estimation. From a practical point of view, among the three methods—minimax design, ED (EID)-optimal, and adaptive design—adaptive design is easiest to implement because of

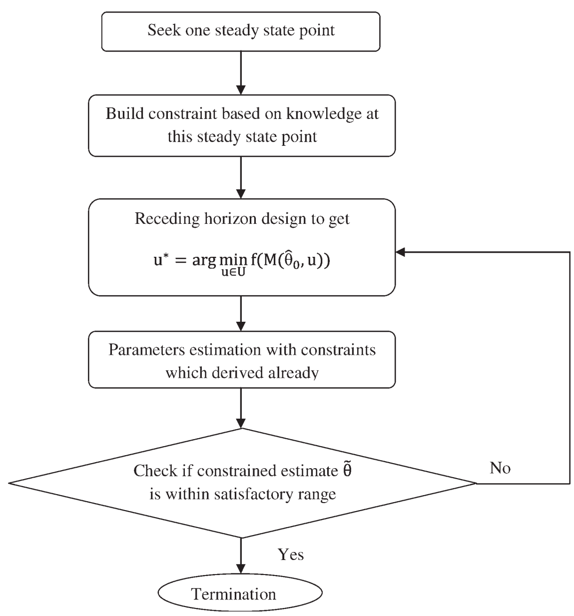

Figure 2. Flow diagram for proposed experiment design.

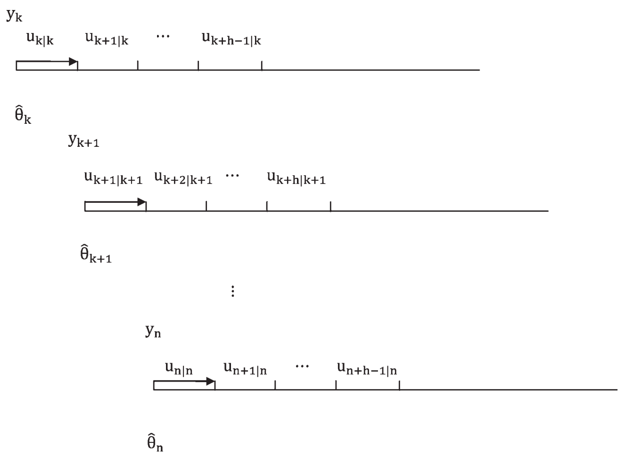

Figure 3. Receding-horizon design.

relatively small computation load and suitability for nonlinear systems. As discussed in the introduction, the main problem with the adaptive design for nonlinear systems is the poor initial values. We will develop a method that provides a solution for dealing with poor initial conditions when applying the adaptive design. The flow diagram of the proposed experiment design is shown first in Figure 2, while the details will be elaborated shortly.

Constructing constraints for parameters

The first step of the proposed design is to impose a constraint according to certain steady-state information. In some cases, steady states can be known *a priori*, whereas in other cases, a simple step test can help determine the steady states. When a steady state is found, it will impose certain constraints on the model parameters. Depending on the characteristics of the individual system, there are two ways to derive the parameter constraints based on the knowledge of steady states. The first method involves directly substituting steady states into the state equation and then equating it to zero. Suppose we have nonlinear state space equation as follows

$$\dot{x}_t = f(\theta, x_t, u_t) + Nw_t \tag{17}$$

$$y_t = x_t + Rv_t \tag{18}$$

where $w_t \sim \mathcal{N}(0, I_{n_x})$, $v_t \sim \mathcal{N}(0, I_{n_y})$, $\mathcal{N}$ stands for Gaussian distribution, n_x and n_y are dimensions of x and y, respectively, and N and R are constant matrices of appropriate dimensions. The steady state is denoted as (x_s, u_s). Substituting this steady-state point into Eq. 17 gives

$$\dot{x} = f(\theta, x_s, u_s) \tag{19}$$

Since $\dot{x} = 0$ at steady state, the following constraint is established

$$g(\theta) = f(\theta, x_s, u_s) = 0 \tag{20}$$

Another approach for specifying constraints is to approximate this nonlinear model at steady state by using a local linear model; these models can be identified by a linear identification algorithm around a steady-state point. For illustration purpose, the electronic circuit system as shown in (7) is used to derive the parameter constraints. With perturbations around a steady state, perform continuous-time system identification,[15] and then the following model is identified

$$\dot{x}_t = -\frac{x_t}{0.001783} + \frac{u_t}{1.1998} \tag{21}$$

$$y_t = x_t \tag{22}$$

A constraint can therefore be set up as

$$\theta_1 \theta_2 = 0.001783 \tag{23}$$

Note that because of unavoidable estimation error in identification, this constraint is an approximate one.

Obviously, additional steady states can be found from step response tests. Notice that more constraints are incorporated, the narrower range of parameter estimate can be. For simplification, we adopt only one constraint derived from one steady state in the examples. For additional steady-state conditions, the proposed algorithm can also be applied in the same manner.

Receding-horizon design

Stigter et al.[8] proposed an adaptive approach for experiment design with a receding-horizon idea. Jayasankar et al.[16] later formalized the design and called it as a receding-horizon experiment design. In receding-horizon design, the optimization is performed to obtain U_k^* according to the following equation

$$U_k^* = [u_{k|k}^* \; u_{k+1|k}^* \; \cdots \; u_{k+h-1|k}^*] = \arg\min_{U_k \in} f(M(\hat{\theta}_k, U_k)) \tag{24}$$

where U_k^* is the optimal input vector containing $u_{k|k}^*, u_{k+1|k}^*, \cdots, u_{k+h-1|k}^*$ calculated at the kth time instant, h is the optimization horizon, $\mathbb{U}$ is the feasible set which U_k^* can be chosen from, f and M are explained in Eq. 13 and 14, respectively, and $\hat{\theta}_k$ is the parameter estimate at time instant k.

The procedure of receding-horizon design is performed as follows: solve the optimal design problem according to an objective function such as Eq. 3 with the current estimate $\hat{\theta}_k$ over a time horizon $[k, k + h - 1]$ to get $u_{k|k}^*$ till $u_{k+h-1|k}^*$; implement $u_k = u_{k|k}^*$ and obtain the sampled output y_{k+1} at time instant t_{k+1}; this new measurement y_{k+1} will be used to update the current estimate from $\hat{\theta}_k$ to $\hat{\theta}_{k+1}$, and repeat the optimal design procedure with this new estimate $\hat{\theta}_{k+1}$. The process is shown below in Figure 3 and will be adopted in this article.

EKF with state constraint

The EKF is a classical state estimator for nonlinear systems. Parameters can also be estimated if we consider parameters as augmented states. As discussed before, reducing $\mathrm{Cov}(\hat{\theta})$ is equivalent to increasing the information in the data. Poor initial conditions can lead to poor experiment

Table 1. Continuous-Discrete Extended Kalman Filter

Model	$\dot{\mathbf{x}}(t) = f(\mathbf{x}(t), u(t), t) + G(t)w(t), w(t) \sim N(0, Q(t))$
	$y_k = h(\mathbf{x}_k) + v_k, v_k\ N(0, R_k)$
Gain	$K_k = P_k^- H_k^T(\widehat{\mathbf{x}}_k^-)[H_k(\widehat{\mathbf{x}}_k^-)P_k^- H_k^T(\widehat{\mathbf{x}}_k^-) + R_k]^{-1}$
	$H_k(\widehat{\mathbf{x}}_k^-) \equiv \frac{\partial h}{\partial \mathbf{x}}\Big\|_{\widehat{\mathbf{x}}_k^-}$
Update	$\widehat{\mathbf{x}}_k^+ = \widehat{\mathbf{x}}_k^- + K_k[y_k - h(\widehat{\mathbf{x}}_k^-)]$
	$P_k^+ = [I - K_k H_k(\widehat{\mathbf{x}}_k^-)]P_k^-$
Propagation	$\dot{\hat{\mathbf{x}}}(t) = f(\hat{\mathbf{x}}(t), u(t), t)$
	$\dot{P}(t) = F(\widehat{\mathbf{x}}(t), t)P(t) + P(t)F^T(\widehat{\mathbf{x}}(t), t) + G(t)Q(t)G^T(t)$
	$F(\widehat{\mathbf{x}}(t), t) \equiv \frac{\partial f}{\partial \mathbf{x}}\Big\|_{\widehat{\mathbf{x}}(t)}$

design as discussed before; therefore, it is natural to impose constraints on the state estimations when using EKF so that the experiment design and parameter estimation will not be unduly influenced by poor initial parameters. Contributions on constrained estimation can be found in Refs. 14, 17 and 18 In this work, EKF with equality constraints is adopted.

For illustration, suppose that we have a nonlinear system with one continuous state and one discrete measurement

$$\dot{x} = f(\theta, x, u) \tag{25}$$

$$y_k = h(x_k) \tag{26}$$

In the following, parameters are considered as augmented states. We use $\mathbf{x}$ to signify the state vector that includes parameters θ

$$\mathbf{x} = \begin{bmatrix} x \\ \theta \end{bmatrix} \tag{27}$$

The unconstrained continuous-discrete EKF is shown in Table 1,[19] where $\hat{x}$ denotes unconstrained state estimate.

Consider that the model described by Eqs. 25 and 26 has the following linear constraint

$$D\mathbf{x}_k = d_k \tag{28}$$

where D is $s \times n_x$ dimensional matrix, and s stands for the number of constraints, n_x stands for the number of states being constrained, and d_k is $s \times 1$ vector. Thus, the problem formulation admits inclusion of multiple constraints. More constraints are incorporated, the narrower region of parameters, and more possible to converge to the true set of parameters.

Based on basic equations shown in Table 1, Simon and Chia[14] derived the EKF with equality constraint as

$$\widetilde{\mathbf{x}}_0 = \widehat{\mathbf{x}}_0 \tag{29}$$

$$\widetilde{\mathbf{x}}_k = \widehat{\mathbf{x}}_k - W^{-1}D^T(DW^{-1}D^T)^{-1}(D\widehat{\mathbf{x}}_k - d_k) \tag{30}$$

following the projection method, where W is any symmetric positive-definite weighting matrix. In Eqs. 29 and 30, we have used $\tilde{x}$ to denote constrained state estimate. Throughout the remainder of this article, a "^" denotes an unconstrained estimate and a "~" denotes a constrained estimate, while a "*" denotes an optimal. Usually, W is set as identity matrix I or P^{-1}, where P is the inverse of the covariance matrix for the unconstrained estimate $\widehat{\mathbf{x}}$ obtained from Table 1.

In most nonlinear systems, the constraint is also nonlinear as in Eq. 20. As an approximation, Eq. [20] can be linearized around the current estimate $\widetilde{\mathbf{x}}_k$ as

$$g(\widetilde{\mathbf{x}}_k) + g'(\widetilde{\mathbf{x}}_k)(\mathbf{x}_{k+1} - \widetilde{\mathbf{x}}_k) \approx 0 \tag{31}$$

Then, a linear constraint having the form of Eq. 28 is obtained

$$g'(\widetilde{\mathbf{x}}_k)\mathbf{x}_{k+1} \approx d_{k+1} - g(\widetilde{\mathbf{x}}_k) + g'(\widetilde{\mathbf{x}}_k)\widetilde{\mathbf{x}}_k \tag{32}$$

where $g'(\widetilde{\mathbf{x}}_k)$ is equivalent to D and $d_{k+1} - g(\widetilde{\mathbf{x}}_k) + g'(\widetilde{\mathbf{x}}_k)\widetilde{\mathbf{x}}_k$ equivalent to d in Eq. 28. Then, according to Eq. 29 and 30, the constrained estimate becomes

$$\widetilde{\mathbf{x}}_0 = \widehat{\mathbf{x}}_0 \tag{33}$$

$$\widetilde{\mathbf{x}}_{k+1} = \widehat{\mathbf{x}}_{k+1} - W^{-1}g'(\widetilde{\mathbf{x}}_k)^T(g'(\widetilde{\mathbf{x}}_k)W^{-1}g'(\widetilde{\mathbf{x}}_k)^T)^{-1}(g'(\widetilde{\mathbf{x}}_k)\widehat{\mathbf{x}}_{k+1} - d_{k+1} + g(\widetilde{\mathbf{x}}_k) - g'(\widetilde{\mathbf{x}}_k)\widetilde{\mathbf{x}}_k) \tag{34}$$

Note that both unscented kalman filter and moving horizon estimation can be applied under this constrained framework for parameter estimation. Their state estimation recursion is analogous to that of constrained EKF.[18]

Both adaptive experiment design and constrained estimation have their own advantages, respectively. Adaptive experiment design has low computation cost and is easy to implement. Constraint estimation can improve the performance of estimation.[14] However, neither one of them individually can address the nonlinear estimation problem under poor initial conditions. In terms of constrained state estimation itself, there is one major difference between Simon and Chia's,[14] method and the proposed method. For the constrained EKF in the proposed method, each current $\widetilde{\mathbf{x}}_k$ is involved in the kth step of recursive estimation, whereas in Simon and Chia's[14] method this $\widetilde{\mathbf{x}}_k$ is obtained by projecting the unconstrained estimate $\widehat{\mathbf{x}}_k$ into the constraint space, but is not involved in the iterative framework of EKF for the next state estimate.

With (33) and (34) being available, we use estimate $\widetilde{\mathbf{x}}$ instead of $\widehat{\mathbf{x}}$ in calculating optimality criterion, and this gives us the optimal input $\tilde{u}^*$ for the constrained optimal design. The following Proposition shows that the constrained design achieves better estimation performance than that of unconstrained design in terms of variance of estimation.

Proposition 4. Denote the parameter estimation under constraint optimal design as $\tilde{\theta}(\tilde{u}^*)$ and the parameter estimation under unconstrained optimal design as $\hat{\theta}(\hat{u}^*)$. Then, the following inequality holds

$$\mathrm{Cov}(\hat{\theta}(\hat{u}^*)) > \mathrm{Cov}(\tilde{\theta}(\tilde{u}^*)) \tag{35}$$

Proof. For any input u, the error between the constrained state estimate $\widetilde{\mathbf{x}}$, unconstrained state estimate $\widehat{\mathbf{x}}$, and the true state value $\mathbf{x}$ has the following relation[14]

$$\mathrm{Cov}(\mathbf{x}-\widetilde{\mathbf{x}}) < \mathrm{Cov}(\mathbf{x}-\widehat{\mathbf{x}}) \tag{36}$$

where the inequality in the form of "$A < B$" indicates that the square matrix $B - A$ is positive definite. According to $\mathbf{x}$ defined in Eq. 27, partition

$$A = \mathrm{Cov}(\mathbf{x}-\widehat{\mathbf{x}}) - \mathrm{Cov}(\mathbf{x}-\widetilde{\mathbf{x}}) \tag{37}$$

$$= \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \tag{38}$$

then

$$A_{11} = \mathrm{Cov}(x-\hat{x}) - \mathrm{Cov}(x-\tilde{x}) \tag{39}$$

$$A_{22} = \mathrm{Cov}(\theta-\hat{\theta}) - \mathrm{Cov}(\theta-\tilde{\theta}) \tag{40}$$

$$A_{12} = A_{21}^T \tag{41}$$

$$= E[(x-\hat{x})(\theta-\hat{\theta})^T] - E[(x-\tilde{x})(\theta-\tilde{\theta})^T] \tag{42}$$

The following equations hold

$$\mathrm{Cov}(\theta-\hat{\theta}) = \mathrm{Cov}(\hat{\theta}) \tag{43}$$

$$\mathrm{Cov}(\theta-\tilde{\theta}) = \mathrm{Cov}(\tilde{\theta}) \tag{44}$$

As A is positive definite, A_{22} is positive definite too, i.e., $A_{22} > 0$. In view of (43) and (44), this means $\forall u$

$$\mathrm{Cov}(\hat{\theta}(u)) > \mathrm{Cov}(\tilde{\theta}(u)) \tag{45}$$

where $\hat{\theta}(u)$ [or $\tilde{\theta}(u)$] elaborates that $\hat{\theta}$ (or $\tilde{\theta}$) is an estimate according to the input u. Therefore, the following two inequalities should hold

$$\mathrm{Cov}(\hat{\theta}(\hat{u}^*)) > \mathrm{Cov}(\tilde{\theta}(\hat{u}^*)) \tag{46}$$

$$\mathrm{Cov}(\hat{\theta}(\tilde{u}^*)) > \mathrm{Cov}(\tilde{\theta}(\tilde{u}^*)) \tag{47}$$

where each term represents a different experiment design scheme explained as follows:
$\mathrm{Cov}(\hat{\theta}(\hat{u}^*))$: covariance of unconstrained estimate $\hat{\theta}$ with the optimal input $\hat{u}^*$ based on unconstrained design;
$\mathrm{Cov}(\tilde{\theta}(\hat{u}^*))$: covariance of constrained estimate $\tilde{\theta}$ with the optimal input $\hat{u}^*$ based on unconstrained design;
$\mathrm{Cov}(\hat{\theta}(\tilde{u}^*))$: covariance of unconstrained estimate $\hat{\theta}$ with the optimal input $\tilde{u}^*$ based on constrained design; and
$\mathrm{Cov}(\tilde{\theta}(\tilde{u}^*))$: covariance of constrained estimate $\tilde{\theta}$ with the optimal input $\tilde{u}^*$ based on constrained design.

Among these four covariances, only $\mathrm{Cov}(\hat{\theta}(\hat{u}^*))$ and $\mathrm{Cov}(\tilde{\theta}(\tilde{u}^*))$ are the covariance of the adaptive optimal design schemes without and with constraints, respectively. By optimal design, the following inequalities should hold

$$\mathrm{Cov}(\hat{\theta}(\tilde{u}^*)) > \mathrm{Cov}(\hat{\theta}(\hat{u}^*)) \tag{48}$$

$$\mathrm{Cov}(\tilde{\theta}(\hat{u}^*)) > \mathrm{Cov}(\tilde{\theta}(\tilde{u}^*)) \tag{49}$$

From (46) and (49), we obtain the following result

$$\mathrm{Cov}(\hat{\theta}(\hat{u}^*)) > \mathrm{Cov}(\tilde{\theta}(\tilde{u}^*)) \tag{50}$$

□

Effect of constraints on convergence

In Proposition 4, we show that the estimation covariance with the optimal input $\tilde{u}^*$ obtained from the proposed constrained receding-horizon design (CRHD) is superior to the one with input $\hat{u}^*$ obtained from unconstrained receding-horizon design (URHD) where the constraint is referred to the constraint on the parameters. In this section, we shall discuss performance in terms of convergence.

Lemma 1[9] in the appendices provides a condition for the existence of M iterations after which the estimation can asymptotically converge to the true value in unconstrained case. For constrained case, the number M can be proven to be smaller than that in unconstrained case. In other words, imposing constraints will improve the convergency property. This is shown in Proposition 5 along with its proof in the Appendices.

Remark 1. The poor initial guess can cause problems in parameter estimation including large variance and slow convergence speed. Most of the experiment design algorithms including D-optimality aim at reducing the covariance (variance) of the parameter only. Imposing constraints obviously restricts space of the parameters searching and thus reduces the risk of divergence. As shown in the Proposition 4 in the previous subsection and Proposition 5 in the Appendices, imposing constrains not only improves convergence but also reduces estimation variance.

Uncertainty in constraint

However, there will also be downside of introducing constraint if the constraint is not accurate. Constraint can be corrupted with some uncertainties due to, for example, identification error. This uncertainty in the constraint will lead to an asymptotic bias in the estimation. Take the electrical circuit system in (7) as an example. The constraint as shown in Eq. 23, which is obtained from identification, contains error as the ideal value for the product of θ_1 and θ_2 should be 0.0018. Therefore, if this inaccurate constraint is imposed throughout the whole experiment design and estimation procedure, the convergence of the parameters estimation to the true values will not be possible owing to the inaccurate constraint. To circumvent this problem, one natural option is to release the constraint after certain number of iterations. However, too few steps of estimation with the constraint will not serve the purpose of reducing the effect of poor initial value either. Thus, there is a tradeoff in choosing a proper iteration number between improving the convergence and reducing the estimation bias. The proposition 5 in Appendices has shown that there exists an integer M that constitutes a lower bound on the number of iterations, after which the iteration will converge. This provides a theoretical justification to release constraints after certain steps of iterations.

Remark 2. In practice, to determine when to release the constraints is not difficult. For example, after the estimated parameters have converged within some tolerance, the constraints can be removed and continue for a few more iterations of estimation until further convergence to eliminate possible bias due to inaccurate constraints.

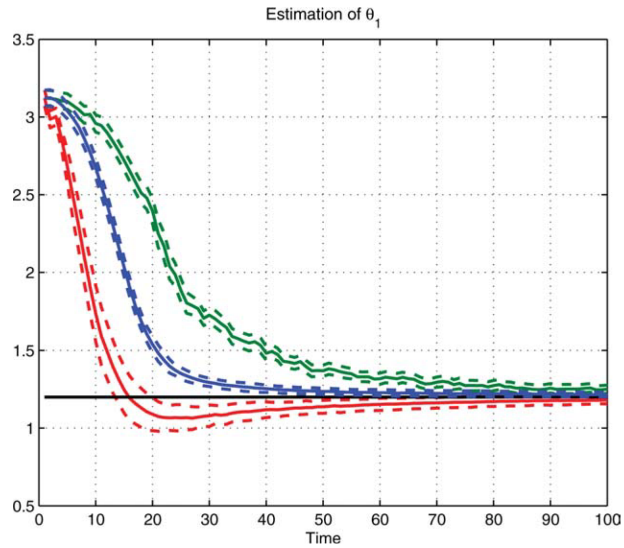

Figure 4. Estimate for parameter θ_1 with deviation (N = 4).

Green: estimation with three-level PRS; blue: unconstraint estimation; red: constraint estimation; dash: standard deviation; and straight black: true value of θ_1. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Examples

In this section, two examples are discussed, one with parameter nonlinearity only, and the other with nonlinearity in both parameters and input. The second example demonstrates the reduction in variance by constrained estimation. From both examples, we can see the advantage of the proposed method in dealing with the poor initial value problem.

The electrical circuit system

The circuit system represented by (7) and (8) is a fast dynamic system with nonlinearity in parameters[12] only. As illustrated in the previous sections, poor initial guess may lead to estimation problems. In this simulation, a poor initial guess is chosen with $E(\hat{\theta}_1^{(0)}) = 3$, $E(\hat{\theta}_2^{(0)}) = 0006$, while the true value is $\theta_1 = 1.2$, $\theta_2 = 0.0015$.

The efficiencies of the multilevel pseudo-random sequences (MLPRSs), unconstrained receding-horizon design (URHD), as well as the proposed constrained receding-horizon design (CRHD) are compared in this example. The efficiency discussed in the following contains two aspects: efficiency of identification and design cost. We will show the identification result under poor initial conditions through the following aspects: the error between the final estimate and the true value, the convergence rate, the standard deviation of each parameter estimate, and the optimality objective function value achieved.

Comparison of simulation results using different design algorithms

MLPRSs are considered as a common input to stimulate a nonlinear system. In this example, we perturb the system by a three-level MLPRS with the values from 2 to 4. The standard deviations for the estimation results in this article are obtained from 30 simulations.

The receding-horizon design has been illustrated in section "Receding-Horizon Experiment Design for Nonlinear System with Poor Initial Conditions." The horizon length is set as $N = 4$.

From Figures 4 and 5, one can see that the proposed CRHD outperforms URHD and MLPRSs in terms of convergence to the true values in the presence of poor initialized conditions. Because θ_2 has larger sensitivity than θ_1, the constrained estimation is more "effective" in θ_2. For the case of unconstrained design, $\hat{\theta}_2$ does not converge. Moreover, one can see from Figure 6 that the constrained design can achieve much smaller objective function value than that of unconstrained design.

CSTR with jacket dynamics

In this example, a continuously stirred tank reactor (CSTR) is used to demonstrate the proposed method when applied to nonlinear chemical processes. The first-order, exothermic reaction $A \rightarrow B$ without recycle is described as follows

$$\dot{c}_A = \frac{q}{V}\left(c_A^f - c_A\right) - k_0 \exp\left(-\left(\frac{E}{R}\right)/T\right)c_A \tag{51}$$

$$\dot{T} = \frac{q}{V}\left(T^f - T\right) + \frac{\Delta H}{\rho C_p} k_0 \exp\left(-\left(\frac{E}{R}\right)/T\right)c_A + \frac{UA}{\rho V C_p}(T_c - T) \tag{52}$$

There are totally eight parameters with two states. The description and nominal value of each parameter are shown in Table 2.[20]

The two states are concentration of component A, c_A, and temperature T. The temperature of cooling jacket T_c is considered as an input.

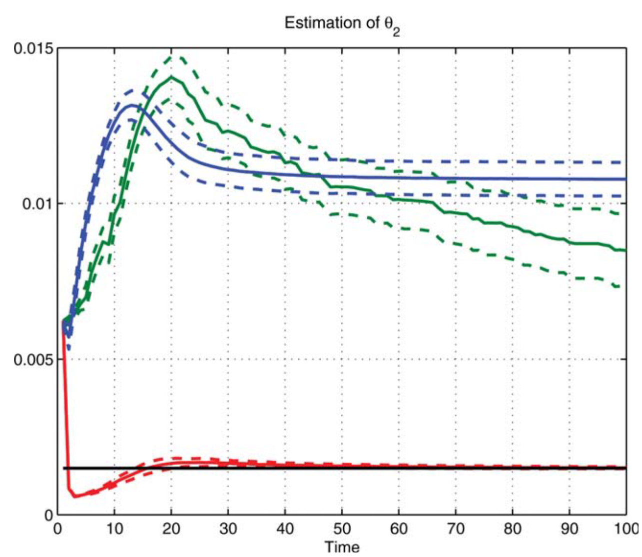

Figure 5. Estimate for parameter θ_2 with deviation (N = 4).

Green: estimation with three-level PRS; blue: unconstraint estimation; red: constraint estimation; dash: standard deviation; straight black: true value of θ_2. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

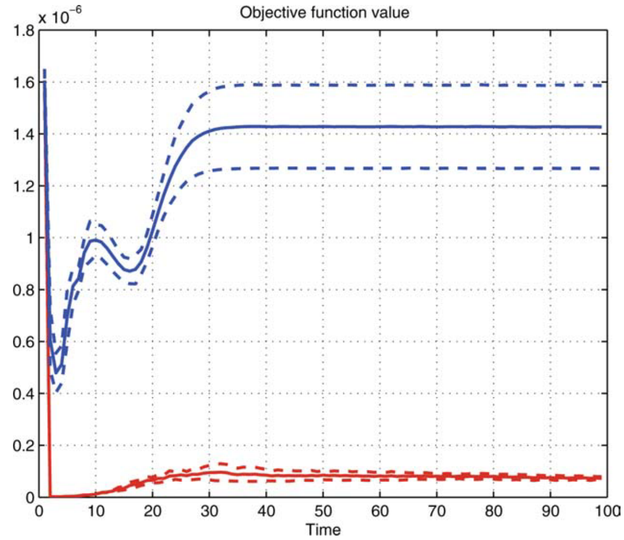

Figure 6. Optimality objective function value.

Upper blue: unconstrained design; bottom red: constrained design; and dash: standard deviation. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Among the large number of parameters shown in Table 2, some are easier to estimate than the others. According to the analysis obtained by Chu et al.,[21] the fluid density ρ and the pre-exponential factor k_0 have larger sensitivities where as activation energy E/R has smaller sensitivity. In the following simulations, both easier-to-estimate and harder-to-estimate sets of parameters are tested using the proposed method.

From a preliminary steady-state test, this CSTR can be determined to have one steady-state point at $c_A = 0.9519$ and $T = 312.7$ when the cooling jacket $T_c = 290$. Substituting this steady-state point into Eq. 52, the constraint equation for each pair of parameters is obtained. To deal with the uncertainty in the constraint, one can release the constraint after some number of iterations as stated in the previous section.

Estimation of ρ and k_0

We start the initial guess of these two easier-to-estimate parameters from relatively poor condition: $E(\rho) = 1000, \sigma(\rho) = 50$, $E(k_0) = 7.3 \times 10^{10}$, and $\sigma(k_0) = 1 \times 10^9$, where σ is standard deviation.

Table 2. Parameters in CSTR

Parameter	Symbol	Value
Density of A-B mixture (kg/m^3)	ρ	1000
Pre-exponential factor (s^{-1})	k_0	7.2×10^{10}
Volumetric flowrate (m^3/s)	q	100
Volume of CSTR (m^3)	V	100
Heat capacity of A-B mixture (J/kg K)	C_p	0.239
Heat of reaction for A-¿B (J/mol)	ΔH	5×10^4
U - overall heat transfer coefficient ($W/m^2\ K$)	UA	5×10^4
A - Area this value is *specific* for the U calculation (m^2)		
Feed concentration (mol/m^3)	c_a^f	1
Feed temperature (K)	T^f	350
E - Activation energy in the Arrhenius equation (J/mol)	$\frac{E}{R}$	8750
R - Universal gas constant = 8.31451 (J/mol / K)		

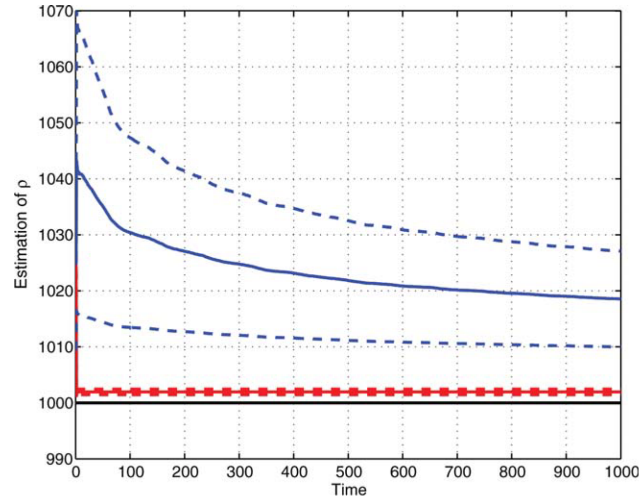

Figure 7. Estimate for ρ with deviation.

Upper blue: unconstraint estimation; bottom red: constraint estimation; dash: standard deviation; and straight black: true value of ρ. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

The parameters estimation result is shown in Figures 7 and 8.

From Figures 7 and 8, one can observe the notable difference between constrained design (constraint is implemented throughout the whole estimation) and unconstrained design in terms of the estimation error and the variance of parameters. This result is consistent with previous simulation example.

As stated before, the steady-state information in this example obtained from step test may not be accurate. In ideal case, the following equation holds

$$g(\theta^0, x_s^0, u_s^0) = 0 \tag{53}$$

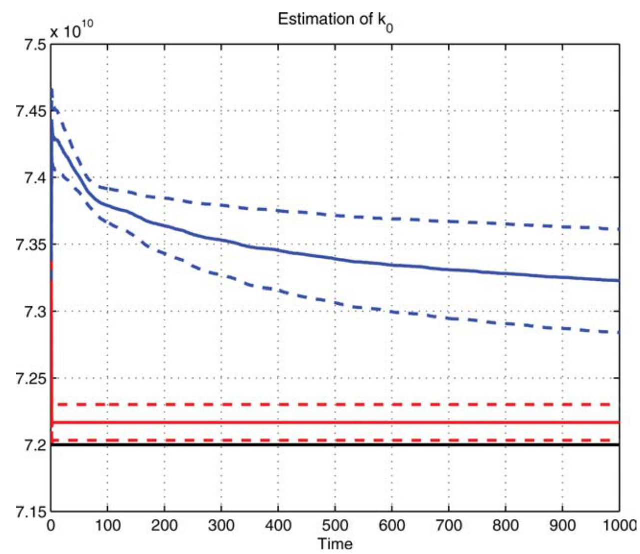

Figure 8. Estimate for k_0 with deviation.

Upper blue: unconstraint estimation; bottom red: constraint estimation; dash: standard deviation; and straight black: true value of k_0. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

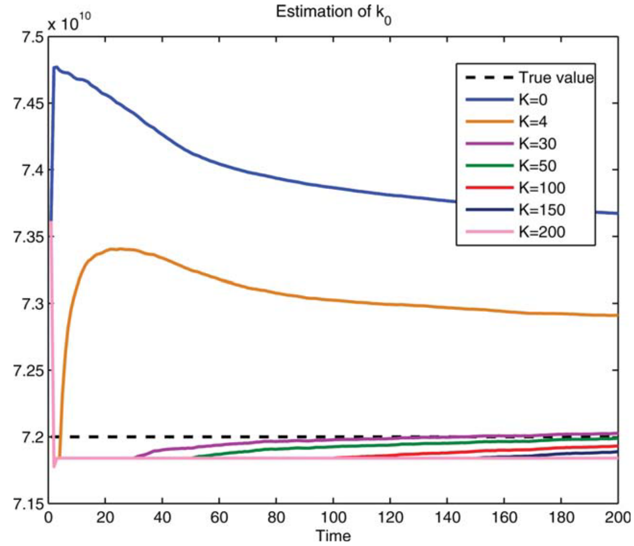

Figure 9. Estimation for parameter k_0 under different *K*.

The number of time steps when constraints implemented. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

where (x_s^0, u_s^0) is the ideal steady-state point. However, without knowing (x_s^0, u_s^0), $(\hat{x}_s, \hat{u}_s^0)$ will be used in the constraint equation. Therefore, the following equation is obtained

$$\hat{g}(\theta, \hat{x}_s, \hat{u}_s) = 0 \tag{54}$$

Indeed, the error has been introduced into the constraint because of the inaccurate steady-state information. Substitute $(\hat{x}_s, \hat{u}_s^0)$ into the constraint equation with true parameters, the following equation holds

$$g(\theta^0, \hat{x}_s, \hat{u}_s) = -964364 \neq 0 \tag{55}$$

From Eq. 55, one can see that there is an error in the constraint equation. This reflects in Figure 9 that the bias appears when the constraint is imposed throughout the estimation procedure ($K = 200$). This is consistent with the analysis in section "Receding-Horizon Experiment Design for Nonlinear System with Poor Initial Conditions." Results of releasing the imprecise constraint after different iterations K are shown in Figure 9 from which one can find that a value of M within the range from 30 to 50.

Because states and parameters are estimated simultaneously, we can also verify the estimate of the states c_A and T to see whether the proposed method shows any advantage.

As shown in Figure 10, the state estimation by constrained design is closest to the true state.

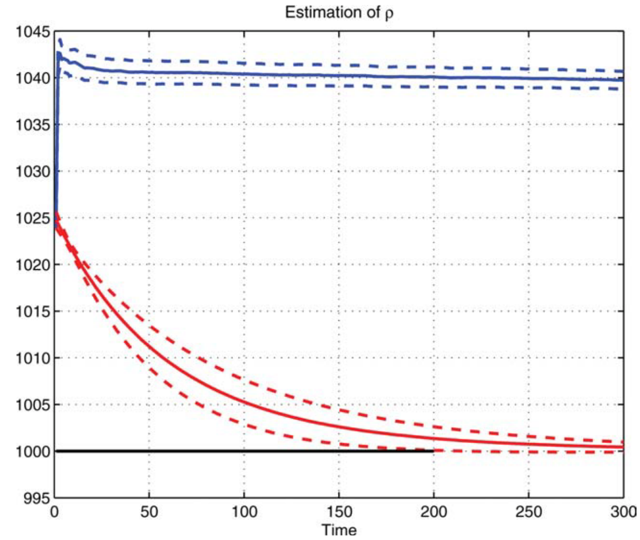

Figure 11. Estimate for ρ with deviation.

Upper blue: unconstraint estimation; bottom red: constraint estimation; dash: standard deviation; and straight black: true value of ρ. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

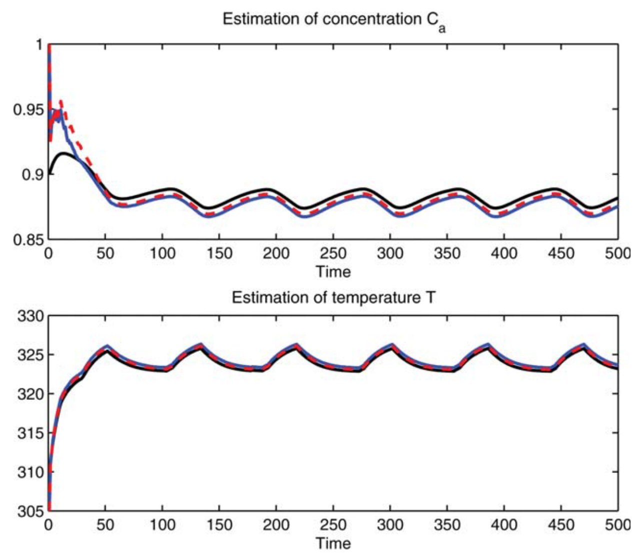

Figure 10. Estimate for c_A (top) and *T* (bottom)

Black: true state value; blue: unconstrained design; and red dash: constrained design. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

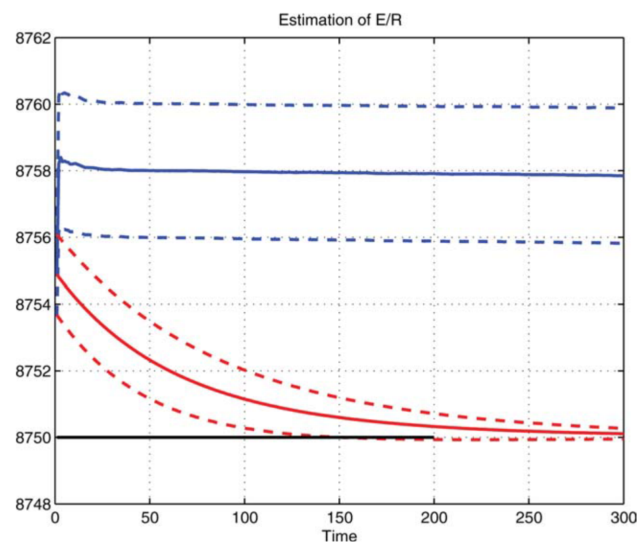

Figure 12. Estimate for *E/R* with deviation.

Upper blue: unconstraint estimation; bottom red: constraint estimation; dash: standard deviation; and straight black: true value of *E/R*. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

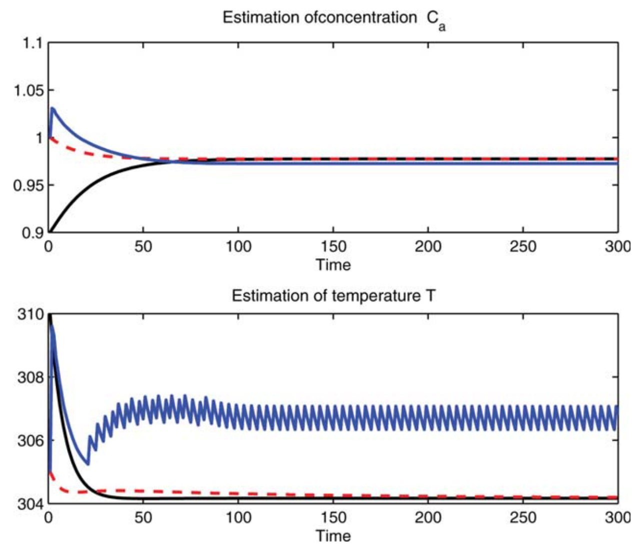

Figure 13. Estimation of state.

Black: true value of state; blue: unconstrained design; red dash: constrained design; upper subplot: estimate of C_a; and bottom subplot: estimate of T. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Estimation of ρ and E/R

Compared to the first set of parameters, this is a set of harder-to-estimate parameters. The initial guesses for the pair of parameters ρ and E/R are chosen as follows: $E(\rho) = 1025$, and $E(E/R) = 8755$. For this set of parameters, constraint is released after 150 iterations. The estimation results are shown in Figures 11 and 12.

From Figures 11 and 12, we can see that both estimated parameters converge to the true values by constrained design but fail to converge with unconstrained design. Moreover, from Figure 13, one can see that the constrained design estimate is closer to the true value comparing to unconstrained design.

Conclusion

A constrained receding-horizon approach for nonlinear dynamic experiment design and parameters estimation was presented, with the purpose of solving problems brought out by poor initial condition. The proposed method incorporated experiment design based on sensitivity analysis and constrained parameter estimation. It is shown that the steady-state condition can be used to form the constraint. It is suggested that when the constraint is not exact, the constraint should be used only for a few iterations in the beginning of the experiment design and parameter estimation and then release after certain steps.

Integration of adaptive experiment design and parameter estimation with constraint proves to be efficient and superior to the unconstrained design. Two simulation examples are used to demonstrate the advantage achieved by the proposed method.

Acknowledgments

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Appendix

Lemma 1 (Observability condition).

Suppose that a nonlinear system described by Eqs. A1 and A2 where w_t and v_t are state noise and output noise, respectively, has the constraint function $g(\theta) = 0$

$$\dot{x}_t = f(\theta, x_t, u_t) + Nw_t \tag{A1}$$

$$y_t = h(x_t) + Rv_t \tag{A2}$$

which satisfies the observability rank condition on a compact subset $K \subset R^n$ (n is the dimension of state). If the estimates of the EKF are sufficiently close to the true state, then the linearized system along the estimated trajectory of the EKF is uniformly observable; i.e., there exist γ_1, γ_2, $1 < \gamma_1 \leq \gamma_2 < \infty$, and $\delta_1 > 0$ such that

$$\gamma_1 I \le O_e^T(X_{n-1}^-, X_{n-2}^+)O_e(X_{n-1}^-, X_{n-2}^+) \le \gamma_2 I \quad \text{(A3)}$$

for all $x_l^- \in K$ such that $|x_l^- - x_l| \le \delta_1$, $l = 0,\ldots, n-1$, and all $x_j^+ \in K$ such that $|x_j^+ - x_j| \le \delta_1$, $j = 0,\ldots, n-2$, and for each $x_0 \in K$, where $x_{l+1} = f(x_l)$, $l = 0,\ldots, n-2$, $X_{n-1}^- \triangleq (x_0^-, \ldots, x_{n-1}^-)$, $X_{n-2}^+ \triangleq (x_0^+, \ldots, x_{n-2}^+)$. "−" and "+" denote "a priori" and "posterior," respectively.

Assumption 2.

1. $A(x) \triangleq \frac{\partial f}{\partial x}(x)$ is invertible at each $x \in R^n$.
2. The following norms are bounded

$$||A|| \triangleq \sup_{x\in R^n} ||A(x)||, \quad ||A^{-1}|| \triangleq \sup_{x\in R^n} ||[A(x)]^{-1}||, \quad \text{(A4)}$$

$$||H|| \triangleq \sup_{x\in R^n} \left|\left| R^{-1}\frac{\partial h}{\partial x}\right|\right|, \quad |||D^2 f||| \triangleq \sup_{x\in R^n} |||D^2 f(x)|||, \quad \text{(A5)}$$

$$|||D^2 h||| \triangleq \sup_{x\in R^n} |||D^2 h(x)||| \quad \text{(A6)}$$

3. Let $g(x,y) \triangleq h(x) - h(y) - \frac{\partial h}{\partial x}(x)(x-y)$, and suppose that there exists $g < \infty$ such that $|g(x,y)| \le g|||D^2h|||x-y|^2$ for all x , $y \in R^n$.

Lemma 3 (Asymptotic observer).

Consider the system in Eqs. A1 and A2 and the EKF framework for the associated noise system. Suppose that Assumption 2 holds. Then, if $|e_k|$, $|||D^2f|||$, and $|||D^2f|||$ are such that for some $\gamma > 0$

$$\varphi(q^{\frac{1}{2}}V^{\frac{1}{2}}(0,e_0), |||D^2f|||, |||D^2h|||) \le -\gamma \quad \text{(A7)}$$

where $e_k = x_k - x_k^-$; p, and q are the corresponding boundaries for error covariance, i.e.,

$$||P_k^{+^{-1}}|| \le p_1 \quad \text{(A8)}$$

$$||P_k^{-^{-1}}|| \le ||P_k^{+^{-1}}|| + ||H||^2 \le p_1 + ||H||^2 \triangleq p \quad \text{(A9)}$$

$$||P_k^+|| \le ||P_k^-|| \le q \quad \text{(A10)}$$

$$q||H||||R^{-1}||^2 \triangleq \delta \quad \text{(A11)}$$

and the following equations are set as follows

$$V(k,e_k) = e_k^T \bar{P}_k^{-1} e_k \quad \text{(A12)}$$

$$\phi(|e_k|, X, Y) \triangleq \delta g Y||A|| + \frac{1}{2}X(pq + \delta g Y|e_k|)^2 \quad \text{(A13)}$$

$$\varphi(|e_k|, X, Y) \triangleq -\frac{1}{rq^2} + p|e_k|\phi(|e_k|, X, Y)\{2pq||A|| + \phi(|e_k|, X, Y)|e_k|\} \quad \text{(A14)}$$

Then the EKF for the noisy system is a local, uniform asymptotic observer for the system in Eqs. A1 and A2.

Lemma 4.

Let $\mathcal{O}$ be a convex compact subset of R^n, $\widetilde{\mathcal{O}}$ the complement of $\mathcal{O}$, and $\varepsilon > 0$ a positive constant. Define $d(x,\widetilde{\mathcal{O}}) = \inf\{|x-y| : y \in \widetilde{\mathcal{O}}\}$, and $\mathcal{O}_\varepsilon = \{x \in \mathcal{O} : d(x,\widetilde{\mathcal{O}}) \ge \varepsilon\}$. Also, assume that

$$\alpha_1 = ||N||^2(1 + ||A||^2 + ||A||^4 + \cdots + ||A||^{2(n-2)}) \quad \text{(A15)}$$

$$\alpha_2 = \lambda_{\min}(NN^T) \quad \text{(A16)}$$

$$a = \max(1, ||A||) \quad \text{(A17)}$$

$$\beta_k = (1 + ||P_0^-||||Dh||^2)a^k \prod_{l=1}^{k} \{1 + ||Dh||^2 \times [||A||^{2l}||P_0^-|| + ||N||^2(||A||^{2(l-1)} + ||A||^{2(l-2)} + \cdots + 1)]\} \quad \text{(A18)}$$

Consider the system in Eqs. A1 and A2 as well as its associated EKF. Suppose that the system satisfies the observability rank condition on a convex compact set $\mathcal{O}$, and that $[\frac{\partial f}{\partial x}]^{-1}$ exists at each $x \in \mathcal{O}$. Let $\delta_1 > 0$ be a constant which satisfies the inequality in Eq. A3 for some $0 < \gamma_1 \le \gamma_2$. Let $p = (\gamma_2 + \frac{1}{\alpha_2})$, $q = a^2(\alpha_1 + \frac{1}{\gamma_1}) + ||N||^2$. Let $\delta_2 > 0$ be such that

$$\varphi((pq)^{1/2}\delta_2, |||D^2f|||, |||D^2h|||) \le -\gamma \quad \text{(A19)}$$

for some $\gamma > 0$, where φ is defined in Eq. A14. Let M be such an integer that when iteration number $k < M$,

$$[1 + (q||A||^2 + ||N||^2)||Dh||^2]||A||(1 + q||Dh||^2) \times \left(1 - \frac{\gamma}{p}\right)^{k/2}(pq)^{1/2} > 1 \quad \text{(A20)}$$

while when $k \ge M$

$$[1 + (q||A||^2 + ||N||^2)||Dh||^2]||A||(1 + q||Dh||^2) \times \left(1 - \frac{\gamma}{p}\right)^{k/2}(pq)^{1/2} < 1 \quad \text{(A21)}$$

Suppose further that $x_k \in \mathcal{O}_\varepsilon$, $k \ge 0$, for some $\varepsilon > 0$, and that $|e_0| \le \frac{\delta}{\beta_n + M - 1}$ with $\delta = \min(\varepsilon/2, \delta_1, \delta_2)$. Then, we have the following result:

1. $|x_k^- - x_k| \le \delta$ and $|x_k^+ - x_k| \le \delta$, $\forall k \ge 0$.
2. The linearized system around x_k^- and x_k^+, i.e., $z_{k+1} = \frac{\partial f}{\partial x}(x_k^+)z_k$, $y_k = \frac{\partial h}{\partial x}(x_k^-)z_k$, satisfies the observability condition in Eq. A3 for $k \ge n-1$. Thus, there exist $q < \infty$, $p < \infty$ such that $\|P_k^-\| \le q$, and $\|P_k^{+-1}\| \le p$, $\forall k \ge n-1$.
3. The error is bounded by δ and converges to zero, i.e., for $k \le n-1$, $|e_k| \le \delta$, and for $k > n-1$, $|e_k| \le \min(\delta, (1 - \frac{\gamma}{p})^{(k-n+1)/2}(pq)^{1/2}\delta)$.

Note: (a) To satisfy the observability condition, it is necessary to keep the estimates x_k^- and x_k^+ near x_k for $0 \le k \le n + M - 1$, thus requiring a good initial guess. (b) We also need to have a converging period ($n - 1 \le k \le n + M - 1$) for the EKF to build up the observability condition; after this, the recursions proceed automatically.

Proposition 5.

Let $\hat{M}$ be the value of M when there is no constraint and $\tilde{M}$ be the value of M when there is constraint. Then, the following inequality holds

$$\tilde{M} \le \hat{M} \quad \text{(A22)}$$

Proof: The condition for existence of M is that there exist γ_1 and γ_2 such that the following inequality holds

$$\gamma_1 I \leq O_e^T(X_{n-1}^-, X_{n-2}^+) O_e(X_{n-1}^-, X_{n-2}^+) \leq \gamma_2 I \quad \text{(A23)}$$

where $X_{n-1}^- \overset{\Delta}{=} (x_0^-, ..., x_{n-1}^-)$, $X_{n-2}^+ \overset{\Delta}{=} (x_0^+, ..., x_{n-2}^+)$. n is the dimension of the state. "$-$" and "$+$" denote "*a priori*" (predicted state) and "*posterior*" (updated state), respectively. The observability matrix O_e in Eq. A23 can be derived by using Lie derivative

$$O_e(x_0^-, x_1^-, x_2^-, x_0^+, x_1^+) = \begin{bmatrix} \frac{\partial h}{\partial x}(x_0^-) \\ \frac{\partial h}{\partial x}(x_1^-)\frac{\partial f}{\partial x}(x_0^+) \\ \frac{\partial h}{\partial x}(x_2^-)\frac{\partial f}{\partial x}(x_1^+)\frac{\partial f}{\partial x}(x_0^+) \end{bmatrix} \quad \text{(A24)}$$

$$= \begin{bmatrix} \frac{\partial h}{\partial x}(x_0^-) \\ \frac{\partial h}{\partial x}(x_1^-)A(x_0^+) \\ \frac{\partial h}{\partial x}(x_2^-)A(x_1^+)A(x_0^+) \end{bmatrix} \quad \text{(A25)}$$

where h is the function defined in (5) and $A = \frac{\partial f}{\partial x}$ is the linearized system function. For Eq. A23 to hold, the boundaries γ_1 and γ_2 on $J_e(X_{n-1}^-, X_{n-2}^+)O_e^T(X_{n-1}^-, X_{n-2}^+)$ $O_e(X_{n-1}^-, X_{n-2}^+)$ (cf. Eq. A3 in Appendix for detail) should exist.

Define that the "*a priori*" estimate x^- is within the range $\underline{x}^- \leq x^- \leq \bar{x}^-$, *the posteriori* estimate x^+ is within the range $\underline{x}^+ \leq x^+ \leq \bar{x}^+$. The boundaries of J_e (if exist) in Eq. A23 can be defined by

$$\hat{\gamma}_1 = \min_{\substack{\underline{x}^- \leq x^- \leq \bar{x}^- \\ \underline{x}^+ \leq x^+ \leq \bar{x}^+}} \lambda_{\min}\{J_e\} \quad \text{(A26)}$$

$$\hat{\gamma}_2 = \max_{\substack{\underline{x}^- \leq x^- \leq \bar{x}^- \\ \underline{x}^+ \leq x^+ \leq \bar{x}^+}} \lambda_{\max}\{J_e\} \quad \text{(A27)}$$

where λ is the eigenvalue of J_e.

With the constraint being imposed, the new boundaries with the constraints can be defined by

$$\tilde{\gamma}_1 = \min_{\substack{\underline{x}^- \leq x^- \leq \bar{x}^- \\ \underline{x}^+ \leq x^+ \leq \bar{x}^+ \\ g(\theta)=0}} \lambda_{\min}\{J_e\} \quad \text{(A28)}$$

$$\tilde{\gamma}_2 = \max_{\substack{\underline{x}^- \leq x^- \leq \bar{x}^- \\ \underline{x}^+ \leq x^+ \leq \bar{x}^+ \\ g(\theta)=0}} \lambda_{\max}\{J_e\} \quad \text{(A29)}$$

Clearly, the boundaries of J_e with constraints will be tighter than the ones without constraint, i.e.,

$$\hat{\gamma}_1 \leq \tilde{\gamma}_1 \leq \tilde{\gamma}_2 \leq \hat{\gamma}_2 \quad \text{(A30)}$$

Let M be such an integer that when iteration number $K < M$ (cf. Eq. A20; Ref. 9), the following inequality holds

$$[1 + (q||A||^2 + ||N||^2)||Dh||^2]||A||(1 + q||Dh||^2) \times (1 - \frac{\gamma}{p})^{K/2}(pq)^{1/2} > 1 \quad \text{(A31)}$$

and for $K \geq M$ (cf. Eq. A21; Ref. 9), inequality Eq. A32 holds

$$[1 + (q||A||^2 + ||N||^2)||Dh||^2]||A||(1 + q||Dh||^2) \times (1 - \frac{\gamma}{p})^{K/2}(pq)^{1/2} < 1 \quad \text{(A32)}$$

where the covariance boundaries p and q are defined as follows (cf. Lemma 3[9])

$$||P_k^{+^{-1}}|| \leq p_1 \quad \text{(A33)}$$

$$||P_k^{-^{-1}}|| \leq ||P_k^{+^{-1}}|| + ||H||^2 \leq p_1 + ||H||^2 \overset{\Delta}{=} p \quad \text{(A34)}$$

$$||P_k^+|| \leq ||P_k^-|| \leq q \quad \text{(A35)}$$

Here, P_k^- and P_k^+ denote covariance of "a priori" (predicted;) and "posterior" (updated) state estimate, respectively; N is the noise matrix in system equation (Eq. A1); $\|A\|$ is defined as $\|A\| \sup_{x \in R^n} \|A(x)\|$ (cf. Assumption 2; Ref. 9); h is the output function in Eq. A2, while Dh is the derivative of $h(x)$; γ is defined through $\varphi(q^{\frac{1}{2}}V^{\frac{1}{2}}(0, e_0), |||D^2 f|||, |||D^2 h|||) \leq -\gamma$ (cf. Lemma 3).

According to Eq. A32, to ensure convergence after M iterations, the following inequality must hold

$$[1 + (q||A||^2 + ||N||^2)||Dh||^2]||A||(1 + q||Dh||^2) \times (1 - \frac{\gamma}{p})^{M/2}(pq)^{1/2} < 1 \quad \text{(A36)}$$

Let the covariance boundaries p and q satisfy the following equations (cf. Lemma 4; Ref. 9)

$$p = \left(\gamma_2 + \frac{1}{\alpha_2}\right) \quad \text{(A37)}$$

$$q = a^2\left(\alpha_1 + \frac{1}{\gamma_1}\right) + ||N||^2 \quad \text{(A38)}$$

where α_1, α_2, and a are defined by the following equations (cf. Lemma 4; Ref. 9),

$$\alpha_1 = ||N||^2(1 + ||A||^2 + ||A||^4 + \cdots + ||A||^{2(n-2)}) \quad \text{(A39)}$$

$$\alpha_2 = \lambda_{\min}(NN^T) \quad \text{(A40)}$$

$$\alpha_2 = \lambda_{\min}(NN^T) \quad \text{(A41)}$$

Denote $\hat{p}$, $\hat{q}$ as the covariance boundaries corresponding to $\hat{\gamma}_1$ and $\hat{\gamma}_2$ when no constraints are imposed, while $\tilde{p}$, $\tilde{q}$ be the covariance boundaries corresponding to $\tilde{\gamma}_1$ and $\tilde{\gamma}_2$ when constraints are imposed. From Eqs. A30, A37, and A38, we have

$$\tilde{p} \leq \hat{p} \quad \text{(A42)}$$

$$\tilde{q} \leq \hat{q} \quad \text{(A43)}$$

Thus

$$1 + (\tilde{q}||A||^2 + ||N||^2)||Dh||^2 \leq 1 + (\hat{q}||A||^2 + ||N||^2)||Dh||^2 \quad \text{(A44)}$$

$$1 + \tilde{q}||Dh||^2 \leq 1 + \hat{q}||Dh||^2 \quad \text{(A45)}$$

$$(\tilde{p}\tilde{q})^{1/2} \leq (\hat{p}\hat{q})^{1/2} \quad \text{(A46)}$$

Notice that here in Eq. A36, $\|A\|$, $\|N\|$, and $\|Dh\|$ are fixed once the system is given. Define μ as

$$\mu = [1 + (q||A||^2 + ||N||^2)||Dh||^2]||A||(1 + q||Dh||^2)(pq)^{1/2} \tag{A47}$$

Using Eqs. A44–A47, we have

$$\tilde{\mu} \leq \hat{\mu} \tag{A48}$$

where $\tilde{\mu}$ is defined when $\tilde{p}$ and $\tilde{q}$ are used in Eq. A47; $\hat{\mu}$ is defined when $\hat{p}$ and $\hat{q}$ are used in Eq. A47.

Considering Eq. A36 and the definition of μ in Eq. A47, one can obtain the following inequalities

$$\left(1 - \frac{\gamma}{\tilde{p}}\right)^{\tilde{M}/2} \tilde{\mu} < 1 \tag{A49}$$

$$\left(1 - \frac{\gamma}{\hat{p}}\right)^{\hat{M}/2} \hat{\mu} < 1 \tag{A50}$$

In addition, we have $\left(1 - \frac{\gamma}{p}\right) < 1$ and $\mu \geq 1$, which can be inferred from Lemma 4[9]. Take logarithm from both sides of (A49) and (A50), it follows clearly that

$$\tilde{M} > 2\log_{(1-\frac{\gamma}{\tilde{p}})} \frac{1}{\tilde{\mu}} \tag{A51}$$

$$\hat{M} > 2\log_{(1-\frac{\gamma}{\hat{p}})} \frac{1}{\hat{\mu}} \tag{A52}$$

From (A42) and Eq. A48, we have

$$\left(1 - \frac{\gamma}{\tilde{p}}\right) \leq \left(1 - \frac{\gamma}{\hat{p}}\right) \tag{A53}$$

$$\frac{1}{\tilde{\mu}} \geq \frac{1}{\hat{\mu}} \tag{A54}$$

From the monotony of logarithm with the base less than 1, one can get the following inequality

$$\log_{(1-\frac{\gamma}{\tilde{p}})} \frac{1}{\tilde{\mu}} \leq \log_{(1-\frac{\gamma}{\tilde{p}})} \frac{1}{\hat{\mu}} \leq \log_{(1-\frac{\gamma}{\hat{p}})} \frac{1}{\hat{\mu}} \tag{A55}$$

This leads to

$$\tilde{M} \leq \hat{M} \tag{A56}$$

where the equality holds only when equalities hold in Eq. A30. ■

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