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Parameter Estimation and Model Discrepancy in Control Systems with Delays

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Abstract: In this paper we consider the problems of parameter estimation and model discrepancy for control systems governed by differential equations. We consider the case where one assumes both modeling and measurement errors. Modeling errors are an important source of model discrepancy which can greatly limit the usefulness of a model for prediction and design. Although Bayesian analysis is a powerful method for dealing with model discrepancy, it is well known that this approach tends to be very sensitive to prior assumptions about the model bias. We present an approach based on science based hierarchical modeling with uncertain disturbances to help develop prior knowledge about model discrepancy in order to improve the model's predictive usefulness. We apply these ideas to examples involving control systems defined by ordinary differential and delay differential equations to illustrate the ideas and suggest future area of research.

Keywords: Delay Differential Equations, Identification, Model Discrepancy.

1. INTRODUCTION AND MOTIVATION

We consider a parameter identification problem for models of physical systems where there are both measurement errors and model discrepancy. A typical approach is to formulate a parameter calibration problem in terms of a nonlinear regression model

$$y(t,q) = g(t,q) + \varepsilon(t)$$

where $y(t)$ is the measured output to the model $g(t,q)$ of the physical system, $\varepsilon(t)$ is a measurement error and $q \in \mathbb{R}^k$ is the model parameter. Assume that $\hat{q}$ is the true value of the calibration parameter and one has M observations which yields the data points

$$\bar{\boldsymbol{y}}_i \triangleq y(\hat{t}_i, \hat{q}) = g(\hat{t}_i, \hat{q}) + \varepsilon(\hat{t}_i)$$

at times $0 \leq \hat{t}_1 < \hat{t}_2 < \hat{t}_3 < \ldots < \hat{t}_{M-1} < \hat{t}_M = T$ on the interval $[0,T]$. In addition to the measurement errors there are possible model discrepancy errors so that

$$g(t,q) = c(t,q) + \delta(t,q) \tag{1}$$

and

$$y(t,q) = c(t,q) + \delta(t,q) + \varepsilon(t), \tag{2}$$

where $c(t,q)$ is the "computed value of the model" and $\delta(t,q) = g(t,q) - c(t,q)$ is the model discrepancy. One source of model discrepancy is numerical errors due to the approximations used to evaluate the model $g(t,q)$. In this case the model discrepancy is sometimes called the simulation error. However, model discrepancy can also be caused by "un-modeled dynamics" or by making incorrect (or simplifying) assumptions about the physical system. In any case, one is led to a regression model

$$y(\hat{t}_i, q) = c(\hat{t}_i, q) + \delta(\hat{t}_i, \hat{q}) + \varepsilon(\hat{t}_i) \tag{3}$$

and the goal is to estimate the unknown parameter $\hat{q} \in \mathbb{R}^k$ in this model from the observed data $\bar{\boldsymbol{y}}_i$.

Model discrepancy in this form was first discussed as a source of uncertainty in numerical simulations in Kennedy and O'Hagan [2001] where $\delta(t)$ is considered as a model bias and analyzed by using a Bayesian approach. Since then much of the literature on model discrepancy has been focused on Bayesian methods (see Arendt et al. [2012a], Arendt et al. [2012b], Bayarri et al. [2007], Bayarri et al. [2009], Brynjarsdottir and O'Hagan [2013], Conti and O'Hagan [2010], Nott et al. [2013], O'Hagan [2006] and Pederson and Johnson [1990]). In this setting one must estimate both the parameter $\hat{q}$ and the model discrepancy term $\delta(t,\hat{q})$. As noted in Bayarri et al. [2007] the discrepancy term $\delta(t,\hat{q})$ is estimated by using approximations of the form

$$\delta(t,\hat{q}) \approx \sum_{j=1}^{N} \beta_j \delta_j(t)$$

where there is considerable freedom in choosing the form of the basis functions $\delta_j(\cdot)$ The parameters β_j are called hyperparameters and are to be estimated along with $\hat{q}$. In the examples below we use polynomials so that

$$\delta(t,\hat{q}) \approx \sum_{j=1}^{N} \beta_j t^{j-1}. \tag{4}$$

The paper Brynjarsdottir and O'Hagan [2013] and the book Smith [2013] provide nice descriptions of this approach. As noted in Bayarri et al. [2007] and Brynjarsdottir and O'Hagan [2013] when applying Bayesian analysis to this problem it is important to use as much information as possible to place prior distributions on q and $b(\cdot)$. In particular, one should use "expert knowledge" about the physical system and its modeling to construct a tight prior distribution for the parameter q. Also, it is suggested that the prior distribution on $\delta(\cdot)$ should "encourage"

$\delta(\cdot) = 0$ so that if one has a perfect simulator there should be a small bias. Finally, since the posterior distributions of q and $\delta(\cdot)$ will typically be highly correlated and sensitive to the priors, using the identified model for prediction in new regions (e.g., to $t > T$) is problematic (see Bayarri et al. [2007]).

In this paper we consider a specific class of problems where expert knowledge about the system dynamics is critical and the model discrepancy is due to modeling the system disturbances. In particular, we assume the physical system is modeled by a delay differential equation of the form

$$\dot{x}(t) = \mathbf{A}_0(q)x(t) + \mathbf{A}_1(q)x(t-r) + \mathbf{G}(q)\omega(t), \quad (5)$$

with initial data

$$x(0) = \eta, \;\; x(s) = \varphi(s), \quad -r \le s < 0, \quad (6)$$

where, $\mathbf{A}_0(q)$, $\mathbf{A}_1(q)$ belong to $\mathbb{R}^{n\times n}$, $\mathbf{G}(q) \in \mathbb{R}^{n\times l}$, $\eta \in \mathbb{R}^n$ and $\varphi(\cdot) \in L^2(-r, 0; \mathbb{R}^n)$. The model output is given by

$$y(t) = \mathbf{C}x(t) + \epsilon(t), \quad (7)$$

where $\mathbf{C} \in \mathbb{R}^{p\times n}$, $\epsilon(t)$ is sensor noise and q is a parametrization of the system matrices. The term $\mathbf{G}(q)\omega(t)$ represents a system disturbance and we shall be interested in the cases where $\omega(t) = 0$ and $\omega(t) \neq 0$.

Consider the special case where $\mathbf{A}_1(q) = 0$ so that (5)-(7) is the ordinary differential equation

$$\dot{x}(t) = \mathbf{A}_0(q)x(t) + \mathbf{G}(q)\omega(t) \quad (8)$$

with initial data

$$x(0) = \eta \in \mathbb{R}^n \quad (9)$$

and output

$$y(t) = \mathbf{C}x(t) + \epsilon(t). \quad (10)$$

The Variation of Parameters Formula implies that

$$x(t) = e^{\mathbf{A}(q)t}\eta + \int_0^t e^{\mathbf{A}(q)(t-s)}\mathbf{G}(q)\omega(s)ds$$

so that

$$y(t, q) = \mathbf{C}e^{\mathbf{A}(q)t}\eta + \int_0^t \mathbf{C}e^{\mathbf{A}(q)(t-s)}\mathbf{G}(q)\omega(s)ds + \epsilon(t). \quad (11)$$

If one assumes that the model has no disturbances, i.e. $\omega(t) = 0$, then the hypothesized regression model is

$$y(t, q) = g(t, q) + \epsilon(t) = \mathbf{C}e^{\mathbf{A}(q)t}\eta + \epsilon(t).$$

On the other hand if $\omega(t) \neq 0$, then the model becomes

$$y(t, q) = c(t, q) + \delta(t, q) + \epsilon(t),$$

where

$$c(t, q) = g(t, q) = \mathbf{C}e^{\mathbf{A}(q)t}\eta$$

and

$$\delta(t, q) = \int_0^t \mathbf{C}e^{\mathbf{A}(q)(t-s)}\mathbf{G}(q)\omega(s)ds. \quad (12)$$

In this formulation the model discrepancy is due to un-modeled disturbances that the model assumed to be zero. Observe that if there is no disturbance so that $\omega(\cdot) = 0$, then $\delta(t, q) = 0$. Moreover, if one assumes a prior distribution on $\omega(\cdot)$, then the model discrepancy due to this disturbance is given by the Variation of Parameters Formula (12) and hence provides specific knowledge about the distribution of $\delta(t, q)$. We will return to this point later and discuss its relationship to the pedagogic example in Bayarri et al. [2007].

2. STATE SPACE FORMULATION OF THE DDE SYSTEM

We use the standard distributed parameter formulation of the DDE system as a system on the Hilbert space $\mathcal{Z} = \mathbb{R}^n \times L^2((-r, 0); \mathbb{R}^n)$ (see Banks and Kappel [1979], Banks et al. [1981], Bensoussan et al. [1992a], Bensoussan et al. [1992b], Burns and Cliff [1981], Cliff and Burns [1982]. We fix $r > 0$ and let

$$D(\mathcal{A}(q)) = \left\{ \begin{bmatrix} \eta \\ \varphi(\cdot) \end{bmatrix} \in \mathbb{R}^n \times H^1((-r, 0); \mathbb{R}^n) : \varphi(0) = \eta \right\} \quad (13)$$

and for $\boldsymbol{z} = [\, \eta \;\, \varphi(\cdot) \,]^T \in D(\mathcal{A}(q))$

$$\mathcal{A}(q)\boldsymbol{z} = \mathcal{A}(q) \begin{bmatrix} \eta \\ \varphi(\cdot) \end{bmatrix} = \begin{bmatrix} \mathbf{A}_0(q)\varphi(0) + \mathbf{A}_1(q)\varphi(-r) \\ \frac{d}{ds}\varphi(\cdot) \end{bmatrix}. \quad (14)$$

Also, define the operator $\mathcal{G}(q) : \mathbb{R}^l \to \mathcal{Z}$ by

$$\mathcal{G}(q)\omega = [\, \mathbf{G}(q)\omega \;\; 0 \,]^T \in \mathcal{Z} = \mathbb{R}^n \times L^2((-r, 0); \mathbb{R}^n) \quad (15)$$

and observe that the DDE system is equivalent to the system

$$\dot{\boldsymbol{z}}(t) = \mathcal{A}(q)\boldsymbol{z}(t) + \mathcal{G}(q)\omega(t). \quad (16)$$

It is well known (see Banks and Kappel [1979], Banks et al. [1981], Burns and Cliff [1981], Cliff and Burns [1982]) that $\mathcal{A}(q)$ generates a C_0-semigroup $S(t, q)$ on $\mathcal{Z}$ and the Variation of Parameters Formula holds. In particular, for $\boldsymbol{z}_0 = [\, \eta \;\, \varphi(\cdot) \,]^T$ it follows that

$$\boldsymbol{z}(t) = S(t, q)\boldsymbol{z}_0 + \int_0^t S(t-s, q)\mathcal{G}(q)\omega(s)ds \quad (17)$$

and

$$S(t, q)\boldsymbol{z}_0 = [\, x(t) \;\, x_t(\cdot) \,]^T,$$

where $x(t)$ is the solution to the DDE system (5)-(6) and $x_t(\cdot) \in L^2((-r, 0); \mathbb{R}^n)$ is the past history function defined by $x_t(s) = x(t+s)$. If $\mathcal{C} : \mathcal{Z} \to \mathbb{R}^p$ is defined by

$$\mathcal{C}\boldsymbol{z} = \mathbf{C}\eta,$$

so that

$$y(t, q) = \mathcal{C}S(t, q)\boldsymbol{z}_0 + \int_0^t \mathcal{C}S(t-s, q)\mathcal{G}(q)\omega(s)ds + \epsilon(t) \quad (18)$$

then the DDE system (5)-(7) is equivalent to the distributed parameter system (16)-(18). Thus again, we have the input-output "regression" model

$$y(t, q) = c(t, q) + \delta(t, q) + \epsilon(t),$$

where

$$c(t, q) = \mathcal{C}S(t, q)\boldsymbol{z}_0$$

and

$$\delta(t, q) = \int_0^t \mathcal{C}S(t-s, q)\mathcal{G}(q)\omega(s)ds. \quad (19)$$

As in the ordinary differential equation problem (8)-(10), the model discrepancy is due to an un-modeled disturbance and the representation (19) provides specific information about how $\delta(t, q)$ inherits its distribution from q and $\omega(\cdot)$. Thus, for problems of this type one can use this prior information to calibrate the model and to improve the model's ability to be predictive for $t > T$.

3. EXAMPLES

We first discuss the pedagogic example presented in Bayarri et al. [2007] where we take the dynamics point of view. Then we turn to a scalar delay differential equation example. Since we begin with a control system with disturbances and the corresponding model discrepancy has a specific representation in terms of q and $\omega(t)$, we can jointly estimate the parameters and the bias term. Moreover, as we show below, the dynamical system approach produces a calibrated model with better predictive properties.

The ODE Example: This model is the same as the pedagogic example in Bayarri et al. [2007]. In particular, the hypothesized regression model is

$$g(t,q) = e^{qt}5 \tag{20}$$

with unknown parameter q. The problem is motivated by assuming the data have arisen from a chemical reaction process with initial chemical concentration 5 and reaction rate q. The parameter was $\hat{q} = -1.70$ and data was assumed to be given by

$$\bar{\boldsymbol{y}}_i = y(\hat{t}_i, \hat{q}) = e^{\hat{q}\,\hat{t}_i}5 + \epsilon(\hat{t}_i)$$

at times $\hat{t}_i \in [0, 3.0]$. A maximum likelihood fit produced the estimate $\hat{q}_{est} = -0.63$ even though the true value of $\hat{q}$ was $\hat{q} = -1.70$. It was clear that the fit-to-data was not good and a modified F test was used to reject (20). The Kennedy and O'Hagan method described in Kennedy and O'Hagan [2001] was used by introducing a bias function $\delta(t)$ so that the model with model discrepancy was given by

$$y(\hat{t}_i, q) = e^{q\hat{t}_i}5 + \delta(\hat{t}_i) + \epsilon(\hat{t}_i)$$

and now one needs to estimate $\hat{q}$ and $\delta(\hat{t}_i)$. The "true biased model" used to generate the data was

$$\bar{\boldsymbol{y}}_i = y_b(\hat{t}_i, \hat{q}) = e^{\hat{q}\hat{t}_i}5 + 1.5[1 - e^{\hat{q}\hat{t}_i}] + \epsilon(\hat{t}_i) \tag{21}$$

so that the model discrepancy is $\delta(\hat{t}_i, \hat{q}) = 1.5[1 - e^{-\hat{q}\hat{t}_i}]$. The authors noted that this model discrepancy arises from a modeling error where it was not recognized that there would be a residual of the chemical (here, 1.5 units) un-reacted. There are two important observations to be made at this point. First, this is a fairly large "modeling error". For example, consider the ODE model of the chemical reaction given by

$$\dot{x}(t) = \hat{q}x(t) + \hat{\omega}, \tag{22}$$

where $\hat{\omega}$ is a an unknown but constant disturbance in the reaction rate. Assuming $x(0) = 5$, it follows from the Variation of Parameters Formula that

$$x(t) = e^{\hat{q}t}5 + \int_0^t e^{\hat{q}(t-s)}\hat{\omega}ds = e^{\hat{q}t}5 - \frac{\hat{\omega}}{\hat{q}}[1 - e^{\hat{q}t}].$$

In this case, the model discrepancy is given by

$$\delta(t, \hat{q}, \hat{\omega}) = -\frac{\hat{\omega}}{\hat{q}}[1 - e^{\hat{q}t}]$$

and to match the (21) one needs $-\hat{\omega}/\hat{q} = 1.5$. This implies that $\hat{\omega} = -(1.5)\hat{q} = -(1.5)(-1.7) = 2.55$ which is a modeling error of the same order as the parameter $\hat{q} = -1.70$. The second point is that one can use knowledge about the science to attack the model discrepancy in a direct way by formulating the system identification problem as a least squares parameter identification problem for the ODE model. In particular, one can use a least squares method to estimate the two parameters $\hat{q}$ an $\hat{\omega}$ using the ODE model (22). Thus, we are led to two approaches:

[Method 1] Let $\bar{\boldsymbol{y}}_i$ be measured data at times times $0 \le \hat{t}_1 < \hat{t}_2 < \hat{t}_3 < \ldots < \hat{t}_{M-1} < \hat{t}_M = T$ on the interval $[0, T]$. The regression model is assumed to have the form

$$y(\hat{t}_i, q) = e^{q\hat{t}_i}5 + \delta(\hat{t}_i) + \epsilon(\hat{t}_i)$$

with a polynomial expansion of the bias function

$$\delta(t, \hat{q}) \approx \sum_{j=1}^{N} \beta_j t^{j-1}.$$

Solve the least squares problem of minimizing

$$J_1(q, \beta_1, \beta_2, \ldots, \beta_N) = \sum_{i=1}^{M} \left| y(\hat{t}_i, q, \beta_1, \beta_2, \ldots, \beta_N) - \bar{\boldsymbol{y}}_i \right|^2 \tag{23}$$

to estimate the parameter $\hat{q}$ and the hyperparameters β_j, $j = 1, 2, \ldots, N$.

[Method 2] Let $\bar{\boldsymbol{y}}_i$ be measured data at times times $0 \le \hat{t}_1 < \hat{t}_2 < \hat{t}_3 < \ldots < \hat{t}_{M-1} < \hat{t}_M = T$ on the interval $[0, T]$. The dynamic model is defined by the system

$$\dot{x}(t) = qx(t) + \omega, \quad x(0) = 5$$

where ω is a constant but unknown disturbance. The output is given by

$$y(\hat{t}_i, q, \omega) = x(\hat{t}_i) + \epsilon(\hat{t}_i).$$

Solve the least squares problem of minimizing

$$J_2(q, \omega) = \sum_{i=1}^{M} \left| y(\hat{t}_i, q, \omega) - \bar{\boldsymbol{y}}_i \right|^2 \tag{24}$$

to estimate the parameter $\hat{q}$ and the disturbance $\hat{\omega}$.

We will apply both methods to this ODE example and to the DDE example described below.

The DDE Example: We begin with the nonlinear regression model on $[0, 3]$ defined piecewise by (see the Appendix)

$$g(t, q_0, q_1) = \begin{cases} e^{q_0 t}5, \\ e^{q_0 t}5 + q_1 5(t - r)e^{q_0(t-r)}, \\ (5 + q_1 5r)e^{q_0(t-r)} + (q_1 5)(t - 2r)e^{q_0(t-r)} \\ \quad + ((q_1)^2 5)/2)(t - 2r)^2 e^{q_0(t-2r)}, \end{cases} \tag{25}$$

on $[0, r]$, $[r, 2r]$ and $[2r, 3r]$, respectively. Data is generated by the scalar DDE

$$\dot{x}(t) = \hat{q}_0 x(t) + \hat{q}_1 x(t - r) + \hat{\omega} \tag{26}$$

with initial data

$$x(0) = 5, \ x(s) = 0, \ -r \le s < 0 \tag{27}$$

and output

$$y(t, \hat{q}) = x(t) + \epsilon(t). \tag{28}$$

As in the ODE example, we generate data using $\hat{q} = [\hat{q}_0, \hat{q}_1]^T$ and a non-zero constant disturbance $\hat{\omega}$. This provides a discrepancy that is not represented in the model (25). Thus, using Method 1, we would assume that

$$y(\hat{t}_i, \hat{q}) = g(\hat{t}_i, \hat{q}_0, \hat{q}_1) + \delta(\hat{t}_i) + \epsilon(\hat{t}_i),$$

where we approximate the bias term by

$$\delta(t) \approx \sum_{j=1}^{N} \beta_j t^{j-1}$$

and employ a maximum likelihood method to estimate the parameters $\hat{q}_0$ and $\hat{q}_1$ and the hyperparameters β_j. Applying Method 2 would mean using a least squares method to estimate the parameters $\hat{q}_0$ and $\hat{q}_1$ and the disturbance $\hat{\omega}$ by a direct parameter identification algorithm applied to the DDE system (26)-(27). As in Bayarri et al. [2007] the regression model is hypothesized to be the solution of the system (26)-(28) on the interval $[0, 3r]$ with no disturbance (i.e., $\hat{\omega} = 0$). The formula for this model is given in the Appendix.

4. NUMERICAL RESULTS

In this section we apply the two approaches Method 1 and Method 2 to the ODE and DDE models in the previous section. The time interval is $[0, 3r]$ and we generated 151 data points by using the analytic solution and adding normally distributed noise with mean 0 and variance $\sigma^2 = 0.3$. The initial value $\eta = 5$ is used in all runs and for the DDE model we set the delay $r = 1$. For Method 1 we minimized $J_1(\cdot)$ defined by (23) and for Method 2 we minimized $J_2(\cdot)$ defined by (24).

Example 1. This is the ODE example from Bayarri et al. [2007] where we set $\hat{q} = -1.70$ and $\hat{\omega} = .2$ and apply both methods. For Method 1, we used $\delta(t) \approx \beta_1 + \beta_2 t + \beta_3 t^2$ and identified $\hat{q}$ and the three hyperparameters β_1, β_2, and β_3. Applying Method 2 we estimated $\hat{q}$ and the disturbance $\hat{\omega}$. The initial estimate for $\hat{\omega}$ was always taken to be $\omega = 0$ so that the assumption is that there is no disturbance, or equivalently that the hypothesized regression model (20) is valid. Both methods provided produced almost identical least squares fit-to-data on the interval $0 \le t \le 3$. Method 2 produces an estimates of the nonzero disturbance and hence the corresponding bias term. The following table is typical of results for both methods. Observe that if $\beta_2 \neq 0$ or $\beta_3 \neq 0$, then Method 1 produces an unbounded model (i.e., $\lim_{t\to+\infty} |y(t, \hat{q}^{opt})| = +\infty$) and eventually the regression model fails to be a good predictor for $t > 3$. However, Method 2 produces the correct qualitative behavior. The steady state solution $\widehat{xss} = 0.12$ and Method 2 produces an estimate of $\widehat{xss}_e = 0.07$. Of course this single fit-to-data does not provide enough information about the uncertainty in the parameter estimate. Rather than focus on this example, we turn to the DDE example and consider this more in detail.

Method 1

$\hat{q}$	β_1	β_2	β_3
-1.7359	0.1305	0.0287	-0.0179

Method 2

$\hat{q}$	$\hat{\omega}$
-1.6305	0.1134

Example 2. This is the DDE example from above. Here we set $\hat{q}_0 = -1.70$, $\hat{q}_1 = 1.20$ and $\hat{\omega} = .1$ and apply both methods. As before, to apply Method 1, we used $\delta(t) \approx \beta_1 + \beta_2 t + \beta_3 t^2$ and identified $\hat{q}_0$, $\hat{q}_1$ and the three hyperparameters β_1, β_2, and β_3 by minimizing the least squares functional $J_1(\cdot)$ defined by (23). Applying Method 2 we identified $\hat{q}_0$, $\hat{q}_1$and the disturbance $\hat{\omega}$ by minimizing the functional $J_2(\cdot)$ defined by (24). In order to include the effects of numerical approximations we employed the spline method in Banks and Kappel [1979] and Banks et al. [1981] to approximate the dynamical system generated by the DDE model.

The tables below illustrates a typical run. In Figure 1 we see that both methods produce excellent fit-to-data plots. On on the interval $0 \le t \le 3$ the difference between the two models is insignificant. However, as for the ODE example above, Method 1 produces a model that incorrectly predicts unbounded solutions while Method 2 correctly produces a stable model. Recall that the DDE (26) is stable if $\hat{q}_0 < 0$ and $|\hat{q}_1| < -\hat{q}_0$ (see Hale [1971] and Hale [1993]).

Method 1

$\hat{q}_0$	$\hat{q}_1$	β_1	β_2	β_3
-1.7108	1.3453	0.0825	-0.1223	0.0168

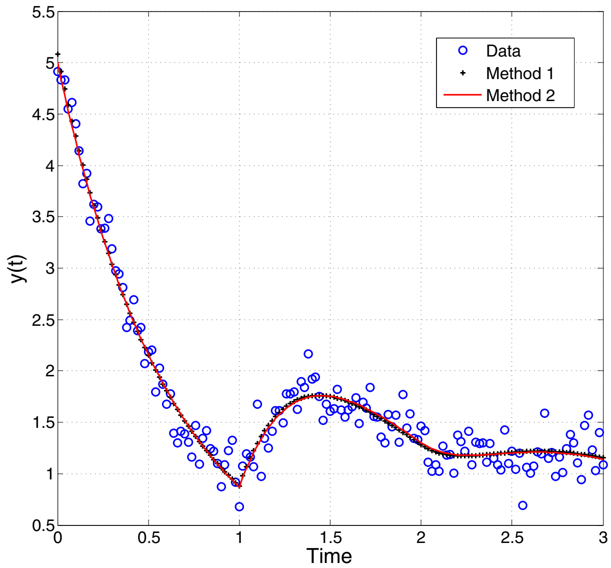

Fig. 1. Example 2: Comparison of Methods for $0 \le t \le 3$

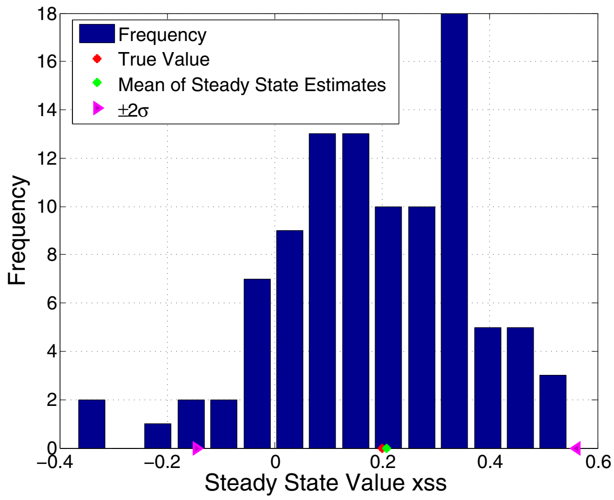

Fig. 2. Example 2: Method 2 - Frequency Plot for xss

Method 2

$\hat{q}_0$	$\hat{q}_1$	$\hat{\omega}$
-1.7387	1.1856	0.1828

In addition, we conducted a simple statistical analysis of Method 2 to see how well the estimated parameters capture the long time behavior of the system. In particular, we assumed the experimental outputs could be repeated to obtain multiple sets of data and used the repeated observations to estimate the parameters. In particular, we generated 5 noisy data sets as above, used Method 2 to estimate the parameters for these 5 cases and then used the mean of these parameter to compute an estimate of the steady state solution for the DDE system. Given a stable DDE system (26), if $q_0 + |q_1| < 0$, then the steady state response is given by

$$xss = \frac{-\omega}{q_0 + q_1},$$

so that when $\hat{q}_0 = -1.70$, $\hat{q}_1 = 1.20$ and $\hat{\omega} = .1$, one has $\widehat{xss} = 0.20$. We also conducted 100 runs with 5 repeated observations for each run. Figure 2 is a frequency plot for this set of simulations. The actual steady state $\widehat{xss} = 0.20$ is

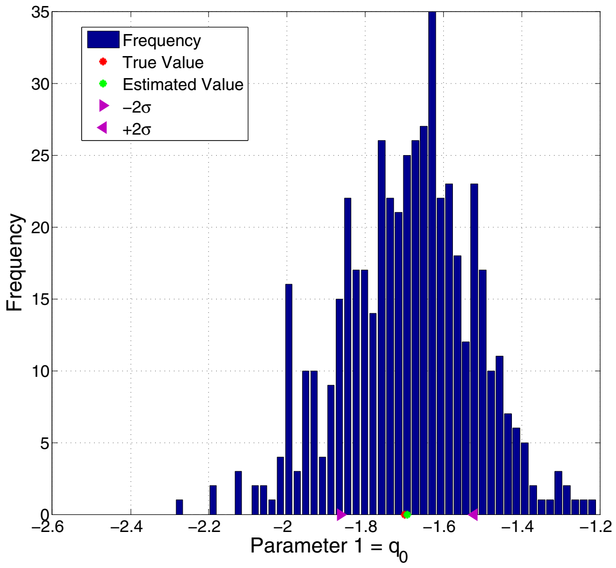

Fig. 3. Example 3: Method 2 - Frequency Plot for q_0

given by the red star on the plot. The mean of the estimated steady states is $\widehat{xss}_e = 0.2083$ and is given by the green star. The triangles are located at $\pm 2\sigma$ from the computed mean $\widehat{xss}_e = 0.2083$. This example illustrates some benefits of using the physics based model described by ODEs or DDEs to provide prior information about model discrepancy.

Example 3. Here we illustrate potential issues when the DDE system (26) is "near" an unstable system. We consider the problem with $\hat{q}_0 = -1.70$, $\hat{q}_1 = 1.65$ and $\hat{\omega} = .2$. Observe that $\hat{q}_0 + |\hat{q}_1| = -0.05$ so that a positive perturbation of $\hat{q}_1$ on the order 0.05 renders the system unstable. We solved 500 least squares estimation problems with new noise added to the data for each run. Figures 3 - 5 are frequency plots for each of the three parameters q_0, q_1 and ω. As one might expect, some estimated parameters produced values of $\hat{q}_0$ and $\hat{q}_1$ satisfying $\hat{q}_0 + \hat{q}_1 > 0$. Although these parameter estimates provide excellent fit-to-data on $0 \leq t \leq 3$, clearly the unstable models fail to predict the long term dynamics. However, of the 500 runs only 3 produced an unstable model. Moreover, these cases do not occur if one uses repeated observations as in the previous example.

5. CONCLUSIONS

We have presented an approach for dealing with certain model discrepancies when the model arises naturally as a physics based model in the form of a dynamical system generated by systems of ODEs and DDEs. Model discrepancy due to modeling uncertainties and/or disturbances can be used as prior knowledge for parameter estimation. In these cases, model prediction outside of the interval for which data was collected can be enhanced.

Method 2 works best when one has a physics based model with reasonable bounds (error bars) on the system parameters. In addition, one can easily constrain the problem by imposing conditions on the parameters such as

$$q_0 < 0,$$

and

$$q_0 + |q_1| < 0,$$

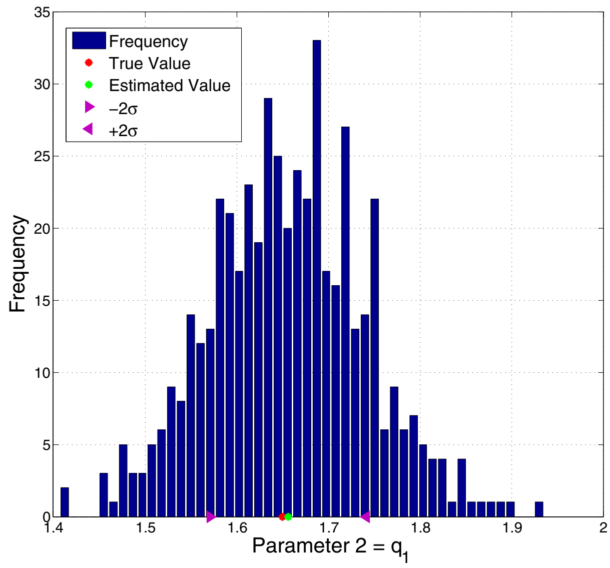

Fig. 4. Example 3: Method 2 - Frequency Plot for q_1

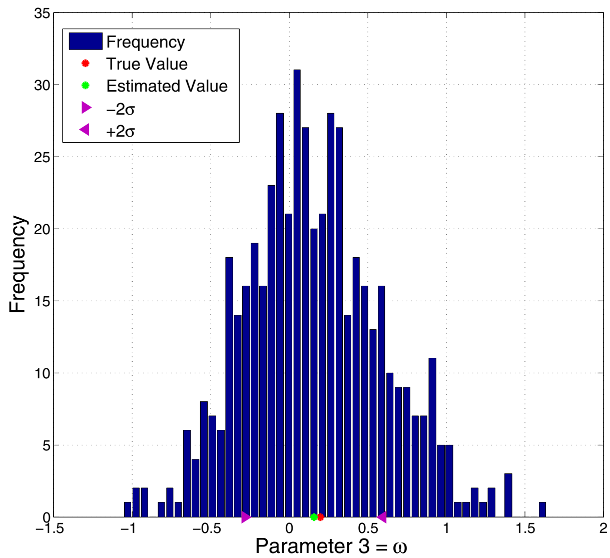

Fig. 5. Example 3: Method 2 - Frequency Plot for ω

to ensure stability. In this case one has a constrained least squares problem.

Method 1 is very general and is the subject of numerous recent research papers (see Arendt et al. [2012a], Arendt et al. [2012b], Bayarri et al. [2007], Bayarri et al. [2009], Brynjarsdottir and O'Hagan [2013], Conti and O'Hagan [2010] and Nott et al. [2013]). Although not fully discussed here Method 1, has a sound theoretical basis in Bayesian statistics. Dealing with the issue of model prediction outside the time interval on which data is available remains an active research area. Of course one would expect that a Bayesian approach would be very useful in cases where one begins with a physics based model and then considers the parameters and disturbances as random parameters.

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6. APPENDIX: EXACT SOLUTION TO THE DDE

The exact solution of the DDE (26)-(27) was computed by the method of steps (see Bellman and Cooke [1963], Hale [1971] and Hale [1993]) on $[0, 3r]$ is given piecewise by

$$x(t) = a_1 e^{q_0 t} + a_2,$$

on $[0, r]$, by

$$x(t) = b_1 e^{q_0 t} + b_2(t - r)e^{q_0 t} + b_3,$$

on $[r, 2r]$ and by

$$x(t) = c_1 e^{q_0 t} + c_2(t - 2r)e^{q_0 t} + c_3(t - 2r)^2 e^{q_0 t} + c_4,$$

on $[2r, 3r]$. Here, the coefficients are

$$\begin{aligned}
a_1 &= a_1(\omega) = \eta + (\omega/q_0),\\
a_2 &= a_2(\omega) = -(\omega/q_0),\\
b_1 &= b_1(\omega) = a_1 + (a_2 + ((q_1 a_2 + \omega)/q_0))e^{(-q_0 r)},\\
b_2 &= b_2(\omega) = q_1 a_1 e^{(-q_0 r)},\\
b_3 &= b_3(\omega) = -(q_1 a_2 + \omega)/q_0,\\
c_1 &= c_1(\omega) = b_1 + b_2 r + b_3 e^{(-q_0 2r)}\\
&\quad + ((q_1 b_3 + \omega)/q_0)e^{(-q_0 2r)},\\
c_2 &= c_2(\omega) = q_1 b_1 e^{(-q_0 r)},\\
c_3 &= c_3(\omega) = (q_1 b_2 e^{(-q_0 r)})/2,\\
c_4 &= c_4(\omega) = -(q_1 b_3 + \omega)/q_0.
\end{aligned}$$

Observe that for $\omega = 0$, it follows that $a_2 = a_2(0) = 0$, $b_3 = b_3(0) = 0$ and $c_4 = c_4(0) = 0$. The remaining non zero coefficients are given by

$$\begin{aligned}
a_1 &= a_1(0) = \eta,\\
b_1 &= b_1(0) = \eta,\\
b_2 &= b_2(\omega) = q_1 \eta e^{(-q_0 r)},\\
c_1 &= c_1(\omega) = \eta + q_1 \eta e^{(-q_0 r)} r,\\
c_2 &= c_2(\omega) = q_1 \eta e^{(-q_0 r)},\\
c_3 &= c_3(\omega) = (q_1)^2 \eta e^{(-q_0 2r)})/2
\end{aligned}$$

and hence $x(t)$ is defined on the intervals $[0, r]$, $[r, 2r]$, $[2r, 3r]$,

$$x(t) = \begin{cases} e^{q_0 t} 5, \\ e^{q_0 t} 5 + q_1 5(t - r)e^{q_0(t-r)}, \\ (5 + q_1 5r)e^{q_0(t-r)} + (q_1 5)(t - 2r)e^{q_0(t-r)} \\ \quad + ((q_1)^2 5)/2)(t - 2r)^2 e^{q_0(t-2r)}, \end{cases}$$

respectively.

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