

A Partial Flatness Approach to Nonlinear Moving Horizon Estimation

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Abstract—Moving horizon estimators based on an optimization formulation have been proposed as an alternative to extended Kalman filters for constrained nonlinear estimation. An efficient approach to the solution of the nonlinear dynamic optimization resulting from the Nonlinear Moving Horizon Estimation (NMHE) problem is presented in this paper. The dynamic optimization problem for the continuous NMHE is transformed into a lower dimensional nonlinear programming problem by eliminating the dynamic constraints for a differentially flat nonlinear system. For the case where the system is not differentially flat, a subset of the nonlinear differential equations can be eliminated. The optimization scheme is demonstrated for the disturbance estimation in a nonlinear chemical reactor.

I. INTRODUCTION

In many chemical engineering processes, the primary variables are controlled and are not measurable. In such cases, secondary variable measurements are often used to infer the primary variables. For a review of nonlinear inferential control, see Doyle III [1]. In addition to the primary variables, it has been observed that estimates of unmeasured disturbances can lead to improved controller performance, when model based schemes such as nonlinear model predictive control are used [2]. Common estimator formulations include the Kalman filter, its nonlinear extensions (*e.g.* Extended Kalman filter), and Luenberger observer. The performance of the Kalman filter has been shown to degrade, when constraints on the estimates and nonlinearities are present [3]. Moving Horizon Estimators (MHE) involving the solution of a dynamic optimization problem have been proposed for such problems to handle the constraints.

A critical issue associated with MHE, particularly for the nonlinear system, is the computational cost associated with the solving the dynamic optimization problem. In this study, an approach based on the structure of the nonlinear process model is proposed for the solution of the MHE optimization problem. The concept of differential flatness, a property of the structure of the nonlinear process model, has been exploited in the past for efficient dynamic optimization in the context of model predictive control problem (the dual of the nonlinear MHE) [4], [5], [6]. The idea has been extended to the control of nonlinear process models that are not differentially flat through a combination of the simultaneous approach [7] and the flatness based

approach [8] (input elimination based approach). Herein, a computationally efficient approach to the MHE problem is proposed and compared to the traditional method based on the simultaneous formulation. The two approaches are demonstrated for disturbance estimation in a chemical reactor.

II. MOVING HORIZON ESTIMATION PROBLEM

Consider a process model of the following form:

$$\begin{aligned}\dot{\mathbf{x}} &= \mathbf{f}(\mathbf{x}, \mathbf{u}, \boldsymbol{\theta}) + \boldsymbol{\omega} \\ \mathbf{y}_k &= \mathbf{h}(\mathbf{x}_k, \boldsymbol{\theta}_k) + \boldsymbol{\nu}_k \\ \mathbf{x}_0 &= \mathbf{x}_0^e + \mathbf{e}_0\end{aligned}\quad (1)$$

where $\mathbf{x} \in \mathbb{R}^n$ is the state vector, $\mathbf{u} \in \mathbb{R}^m$ is the input vector, $\mathbf{y} \in \mathbb{R}^q$ is the output vector, $\mathbf{f} : \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^l \rightarrow \mathbb{R}^n$ and $\mathbf{h} : \mathbb{R}^n \rightarrow \mathbb{R}^q$ are assumed to be smooth vector functions, \mathbf{x}_0^e is the vector of initial state estimate, \mathbf{x}_0 is the actual process initial condition, $\boldsymbol{\theta} \in \mathbb{R}^l$ is the vector of disturbances present in the process, $\boldsymbol{\omega} \in \mathbb{R}^n$ is the vector of errors present in the process model, $\boldsymbol{\nu}$ is the vector of the errors present in the measurement equations, the variables with subscript k refer to the values at a discrete sampling instant (k), and \mathbf{e}_0 is the error in the initial condition estimate. The objective of the MHE is to reconcile the measurements (\mathbf{y}_k) obtained from the process with the dynamic model predictions. In this case, a time window extending from the current instant to a finite time in the past is considered as the estimation horizon. The time profile of the manipulated variable vector (\mathbf{u}), the measurements at the discrete sampling instants and the vector of the initial state estimate (\mathbf{x}_0^e) are known in this horizon. The corresponding dynamic optimization problem is detailed below:

$$\begin{aligned}\text{Max.}_{\boldsymbol{\omega}(t), \boldsymbol{\theta}(t), \mathbf{e}_0, \mathbf{x}(t)} & \quad \left\| P_0^T \mathbf{e}_0 \right\|_2 + \sum_{i=p}^k \left\| R^T \boldsymbol{\nu}_i \right\|_2 \\ & \quad + \int_{t-p\Delta t}^t \left\| Q^T \boldsymbol{\omega} \right\|_2 dt \\ \text{s.t.} & \quad \dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u}, \boldsymbol{\theta}) + \boldsymbol{\omega} \\ & \quad \boldsymbol{\nu}_i = \mathbf{y}_i - \mathbf{h}(\mathbf{x}_i, \boldsymbol{\theta}_i) \\ & \quad \mathbf{e}_0 = \mathbf{x}_0 - \mathbf{x}_0^e\end{aligned}\quad (2)$$

where p is the estimation horizon, P_0 , Q , and R are the vectors of the weights associated with the error in the initial condition, the error in the state equations and the error in the measurement equations, respectively. These weights are tuning parameters in the estimation formulation and can

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be used to represent the relative significance of the model error with respect to the measurement errors. In the current study, it is assumed that model errors can be lumped into a disturbance and thus the focus is on disturbance estimation ($\theta(t) \in \mathbb{R}^l$) hence, the errors in the process model ($\omega(t)$) and the initial condition (e_0) are neglected.

III. SIMULTANEOUS FORMULATION

In the simultaneous formulation, all the states and the disturbance variables are parameterized using orthogonal collocation on finite elements [7]. A notable difference between the NMHE problem and the corresponding control problem (NMPC) is that in the case of NMHE, the manipulated variable profile is known and the decision variables are the states and the disturbance variables. Therefore all the states and the disturbances are parameterized in this approach. The differential equations of the nonlinear process model are imposed at the roots of the orthogonal polynomial through the approximation of the time derivative of the state as a linear combination of the states at specific time instants. The dynamic optimization problem is converted to a nonlinear programming problem (NLP). The mathematical formulation is summarized below:

$$\begin{aligned} \text{Max.}_{\theta(t), \mathbf{x}(t)} \quad & \sum_{i=p}^k \| R^T \nu_i \|_2 \\ \text{s.t.} \quad & A(t_j) \mathbf{X} = \mathbf{f}(\mathbf{x}(t_j), \mathbf{u}(t_j), \boldsymbol{\theta}(t_j)) \\ & \nu_i = \mathbf{y}_i - \mathbf{h}(\mathbf{x}_i, \boldsymbol{\theta}_i) \end{aligned} \quad (3)$$

where $A(t_j)$ is the derivative weight at the time instant (t_j) corresponding to the roots of the orthogonal polynomial in each finite element, t_i is the sampling instant, and \mathbf{X} is the stacked vector of the states at the time instants of parameterization (t_j). Here, $n + l$ variables corresponding to the states and the disturbances are the dynamic decision variables. The number of nonlinear differential equation constraints in this case is n . These are converted into the nonlinear equality constraints in the transformed NLP problem.

IV. FLATNESS BASED FORMULATION

A. Differential Flatness

The idea of differential flatness was first introduced by Fliess and coworkers [9], [10]. This allowed an alternate representation of a system, where trajectory planning and nonlinear controller design become straightforward. These ideas have been applied to a variety of nonlinear systems across the various engineering disciplines for formulating efficient control and optimization algorithms [11], [12], [13], [14]. The definition of the property of differential flatness is given below:

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

A system of ordinary differential equations (4) is said to be differentially flat, if there exist variables (denoted the flat outputs, $\boldsymbol{\xi}$) such that:

- a) These variables are functions of the states, inputs and finite derivatives of the inputs of the form $\xi_i = \zeta_i(\mathbf{x}, \mathbf{u}, \mathbf{u}^{(1)}, \dots, \mathbf{u}^{(\delta)})$, $i = 1, \dots, m$.
- b) All the states and inputs can be expressed in terms of the flat outputs and their derivatives by equations of the type $\mathbf{x} = \chi(\boldsymbol{\xi}, \boldsymbol{\xi}^{(1)}, \dots, \boldsymbol{\xi}^{(\eta)})$ and $\mathbf{u} = \Upsilon(\boldsymbol{\xi}, \boldsymbol{\xi}^{(1)}, \dots, \boldsymbol{\xi}^{(\kappa)})$.
- c) There is no differential equation of the form $\varphi(\boldsymbol{\xi}, \boldsymbol{\xi}^{(1)}, \dots, \boldsymbol{\xi}^{(\rho)}) = 0$. This leads to the restriction that the number of the flat outputs (m) be equal to the number of the manipulated variables.

It should be noted that the vector function \mathbf{f} in equation (4) is assumed to be smooth. The flat outputs and their derivatives provide an alternate representation of the system dynamics such that if the profile of the flat outputs are known as a function of time, then one can obtain the profiles of all the system states and the corresponding inputs. This property is used to calculate the flat output's trajectories. These trajectories are then mapped to the inputs (\mathbf{u}) and the states of the process. It should also be noted that the set of flat outputs and the measured outputs need not have any common elements.

B. Transformed NMHE Formulation

The decision variables in the dynamic optimization problem described in Equation (2) include the process model errors ($\omega(t)$), the disturbances ($\theta(t)$), the states ($\mathbf{x}(t)$) and the initial condition errors (e_0). Here, the process errors are neglected and thus, the dimension of the dynamic decision variables is $l + n$, and the number of nonlinear dynamic equality constraints is n . However, if one can find $\boldsymbol{\xi} \in \mathbb{R}^l$ flat outputs, then the dynamic optimization problem can be transformed using the concept of differential flatness for improved computational efficiency in solving the estimation problem. The transformed optimization problem for NMHE is shown in the following equation:

$$\begin{aligned} \text{Max.}_{\boldsymbol{\xi}(t), \boldsymbol{\psi}(t)} \quad & \| P_0^T e_0 \|_2 \\ & + \sum_{i=p}^k \| R^T \nu_i(\boldsymbol{\xi}, \boldsymbol{\xi}^{(1)}, \dots, \boldsymbol{\xi}^{(\kappa)}) \|_2 \\ \text{s.t.} \quad & c(\boldsymbol{\xi}, \boldsymbol{\xi}^{(1)}, \dots, \boldsymbol{\xi}^{(\kappa)}) \leq 0 \quad \forall t \in [t_0, t_f] \\ & \xi_1^{(r_1)} = \psi_1 \\ & \vdots \\ & \xi_l^{(r_l)} = \psi_l \\ & \boldsymbol{\theta} = \Theta(\boldsymbol{\xi}, \boldsymbol{\xi}^{(1)}, \dots, \boldsymbol{\xi}^{(\tau)}) \\ & \mathbf{x} = \chi(\boldsymbol{\xi}, \boldsymbol{\xi}^{(1)}, \dots, \boldsymbol{\xi}^{(\eta)}) \end{aligned} \quad (5)$$

where ψ_i are the fictitious inputs and are typically parameterized as piece-wise constants, r_i are the controllability indices, c are the nonlinear constraints on the estimated states and $\hat{\boldsymbol{\xi}}$ is the vector of flat outputs, η , and τ are the vector of the highest derivative of the flat outputs that occur in the state and the disturbance transformations, and

Θ and χ are smooth nonlinear functions that transform the flat outputs and their derivatives into the state and the disturbance vector. In this case, the solution of the dynamic equations is obtained through analytic integration of the transformed differential equations as ψ is known. Therefore the nonlinear equality constraints in Equation (3) can be eliminated resulting in computational efficiency. The state and the disturbance profiles are calculated from the flat outputs through the inverse transformation. It should be noted that the flat outputs and their derivatives are obtained through the analytic integration of the dynamic equations in Equation (5), and consequently, the noise in the measured outputs does not lead to amplification in the derivatives of the flat output.

V. INPUT ELIMINATION BASED FORMULATION

A. Input Elimination Based Approach

The approach presented in the previous section was limited to the class of differentially flat nonlinear systems. However, the differential flatness property cannot be rigorously confirmed for an arbitrary nonlinear system. For such systems, the input elimination based approach has been used for formulating efficient algorithms. In this approach, the decision variable in the differential equation is eliminated through rearrangement to obtain the decision variable as a function of the states and their derivatives. The details of this approach for the formulation of efficient algorithms for the Nonlinear Model Predictive Control problem is presented in [8]. A brief summary of the input elimination based approach to dynamic optimization is included below.

In this approach, the inputs are eliminated by using a subset of the dynamic equations to solve for the input transformations. In this case, all the states are chosen as the outputs and one obtains the following set of $n - m$ differential equations:

$$\dot{\hat{\xi}} = f(\hat{\xi}, u, \theta) \quad (6)$$

A subset of the differential equations is chosen and the inputs (the disturbance variables in this case) are expressed in terms of the outputs ($\hat{\xi}$) and their derivatives. Thus, a subset of the dynamic equations are eliminated. The remaining differential equations must be imposed as dynamic equality constraints.

B. Transformed NMHE Formulation

For the estimation problem, the dynamic decision variables are the disturbances and they are eliminated using a part of the model equations. Here, the n states ($\hat{\xi}$) are parameterized and the l disturbances are obtained as a function of the states and their derivatives by rearranging l model differential equations. The remaining $n-l$ differential equations are imposed as nonlinear equality constraints at the roots of the orthogonal polynomial as described in section III. The estimation formulation based on input

elimination is detailed below:

$$\begin{aligned} \text{Max.}_{\xi(t)} \quad & \| P_0^T e_0 \|_2 + \sum_{i=p}^k \| R^T \nu_i(\xi, \xi^{(1)}) \|_2 \\ \text{s.t.} \quad & c(\xi, \xi^{(1)}) \leq 0 \quad \forall t \in [t_0, t_f] \\ & \hat{\xi}_{l+1}^{(r_{l+1})} = \Phi_{l+1}(\xi, \xi^{(1)}) \\ & \vdots \\ & \hat{\xi}_n^{(r_n)} = \Phi_n(\xi, \xi^{(1)}) \\ & \theta = \Xi(\hat{\xi}, \hat{\xi}^{(1)}, \dots, \hat{\xi}^{(\hat{\tau})}) \end{aligned} \quad (7)$$

where $\hat{\tau}$ is the vector of the highest derivative of the flat outputs that occur in the disturbance transformations.

VI. EXAMPLE: NON-ISOTHERMAL VAN DE VUSSE REACTOR

A. Process Model

An extensively studied benchmark problem for nonlinear process control is the van de Vusse kinetic scheme in a continuous stirred tank reactor. The nonlinear process model for a chemical reactor with the van de Vusse reactions are shown below:

$$\begin{aligned} \frac{dC_A}{dt} &= \frac{\dot{V}}{V_R} (C_{AO} - C_A) - k_1(T)C_A - k_3(T)C_A^2 \\ \frac{dC_B}{dt} &= -\frac{\dot{V}}{V_R} C_B + k_1(T)C_A - k_2(T)C_B \\ \frac{dT}{dt} &= \frac{\dot{V}}{V_R} (T_O - T) - \frac{\dot{Q}}{\rho C_p V_R} - \frac{\Delta \hat{H}}{\rho C_p} \\ \Delta \hat{H} &= k_1(T)C_A \Delta H_{RAB} + k_2(T)C_B \Delta H_{RBC} \\ &\quad + k_3(T)C_A^2 \Delta H_{RAD} \\ k_i &= k_{i0} e^{\left(\frac{-E_i}{T+273.15}\right)} \end{aligned} \quad (8)$$

The model parameters used are those presented in Engell and Klatt [15]. The output is the concentration of the product B (C_B) and the input is the rate of energy removed from the reactor (\dot{Q}). The nominal values for the input and the jacket inlet temperature (T_O) are $5.1 kJ/hr$ and $130 C$, respectively. It is assumed that only the reactor temperature is measured every $0.01 hr$. The variation in the jacket inlet temperature is treated as a disturbance. The nonlinear process model is not differentially flat, and therefore the estimation was carried out using the simultaneous and the input elimination based approaches.

In the input elimination based approach, the concentration of reactant (C_A), the concentration of product (C_B), and the temperature of the reactor (T) are the states that are parameterized. The disturbance variable (θ) is then obtained in terms of the parameterized states and the known manip-

ulated variable profile (Q) as shown below:

$$\begin{aligned} \xi &= x \\ \theta &= \left(\dot{\xi}_3 - \Delta H_{Tot} + \frac{\dot{Q}}{\rho C_p V_R} \right) \frac{V_R}{\dot{V}} + \xi_3 - T_O \\ \Delta H_{Tot} &= \frac{k_1 \xi_1 \Delta H_{RAB} + k_2 \xi_2 \Delta H_{RBC} + k_3 \xi_1^2 \Delta H_{RAD}}{\rho C_p} \end{aligned} \quad (9)$$

A term to penalize the changes in the disturbance estimate was incorporated in the objective function to obtain smooth disturbance estimates. The number of the finite elements used in both the cases was 5 and a sixth order Legendre polynomial was used. The input elimination based approach to NMHE is formulated below:

$$\begin{aligned} & \text{Max}_{x(t), u(t)} J(d(t)) \\ &= \sum_{j=0}^p \int_{t-p\Delta t}^t \|\xi_3 - \xi_3^m\|_2 \delta(t - t_j) dt \\ & \quad + w_1 \sum_{j=1}^p \|\theta_j - \theta_{j-1}\|_2 \\ \text{s.t.} \quad & t_j = t - j\Delta t \quad j = 0 \dots p \\ & -30 \leq \theta \leq 30 \text{ K} \quad \forall t_j \\ & \dot{\xi}_1 - \frac{\dot{V}}{V_R} [C_{AO} - \xi_1] + k_1 \xi_1 + k_3 \xi_1^2 = 0 \\ & \dot{\xi}_2 + \frac{\dot{V}}{V_R} \xi_2 - k_1 \xi_1 + k_2 \xi_2 = 0 \end{aligned} \quad (10)$$

Here, $w_1 = 0.001$ is the weight corresponding to the penalty on the rate of change of the disturbance, p is the prediction horizon, $\Delta t = 0.01 \text{ hr}$ is the sample time, ξ_3 is the model prediction of the temperature of the reactor, ξ_3^m is the measured temperature, d_j is the value of the disturbance at the time instant t_j .

TABLE I

COMPARISON OF THE OPTIMIZATION APPROACHES FOR THE SOLUTION OF NMHE PROBLEM

Approach	Number of Parameters	Number of nonlinear equality constraints	CPU time (s) (MATLAB)
Simultaneous	104	63	115
Input Elimination	78	42	45

VII. RESULTS

The results of the estimation using the simultaneous approach and the input elimination based approach are shown in the Figures 1 and 2. The error between the true state and the estimate along with difference between the true state and the state augmented with random noise is depicted

in the figures. The disturbance jacket temperature was assumed to obey a first order response. It was observed that the computational times for the open loop estimation were approximately 115 s and 45 s for the simultaneous and the input elimination based approach, respectively. The details of the NLP problem for NMHE for both the simultaneous and the input elimination based approach are summarized in Table I. The *fmincon* function in MATLAB©(Natick, MA) was used to solve the NLP arising from the transformed NMHE problems. All computations were carried out on a Sun Blade 1000 machine with dual 750 MHz processors. It can be seen from the Figures 1 and 2 that the estimates for both the approaches are similar. It was found that decreasing the penalty on the rate of change of the disturbance resulted in rapid convergence of the estimates to their true values at the cost of increased variability in the estimate. The faster convergence could be the result of the elimination of oscillatory solutions due to the increased penalty. Thus, the input elimination approach for this case seems to be computationally efficient while providing similar results to the simultaneous approach.

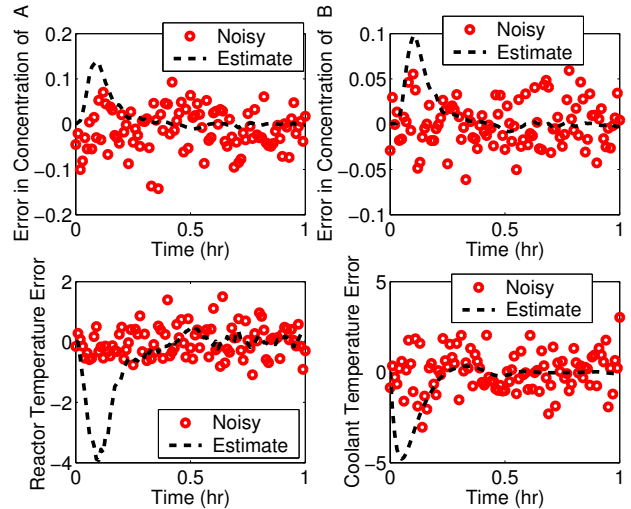


Fig. 1. Estimation results using the simultaneous approach.

VIII. CONCLUSIONS

An efficient algorithm for solving the dynamic optimization associated with the moving horizon estimation is presented. In this approach, the disturbance variables are treated as independent variables, and the input elimination based approach is employed to reduce the number of variables in the optimization problem. This reduction in the problem size leads to computational efficiency in solving the resulting NLP problem. This approach has been successfully employed in the past to address the dynamic optimization problem for the NLMPC problem. Here, a novel method based on the input elimination approach is developed for the efficient solution of the dynamic optimization problem associated with NMHE. This approach is applicable to a

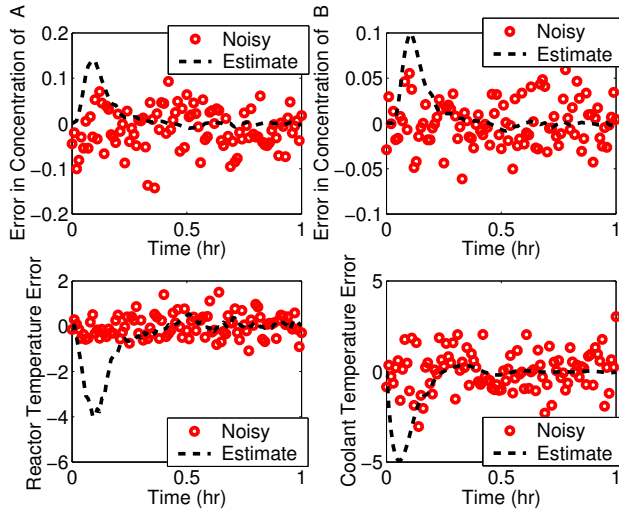


Fig. 2. Estimation results using the input elimination based approach.

general nonlinear system as described by Equation (1). The proposed method is applied for the estimation of the inlet jacket temperature in a chemical reactor with van de Vusse kinetics. The input elimination based approach was compared with the simultaneous approach and was found to be computationally favorable. The example studied here was the problem of a single disturbance estimation that resulted in the elimination of one of the dynamic equation constraints in the input elimination based approach.

Extensions for the case of multiple disturbance would involve the elimination of a larger set of dynamic equality constraints at the cost of potentially increasing the complexity and the nonlinearity of the reduced set of dynamic equations. The current formulation, however, assumes that the process model errors could be lumped into a disturbance variable for estimation. If the estimation formulation is to be extended to the case where process model errors are present, issues related to the non-convexity and convergence to local minima have to be critically examined in the estimation problem, as the solution of the dynamic equations is imposed as the minimization of the objective function. However, when model errors are accounted for, then the number of decision variables available for the optimization increases. Integration of the NMHE with the corresponding Nonlinear Model Predictive Control for improved controller performance is the subject of future investigation.

IX. ACKNOWLEDGEMENT

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