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Model Approximation in Multiparametric Optimization and Control – A Computational Study

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Abstract

Incorporating a high fidelity model that accurately describes a dynamical system in an optimization and control study may often lead to an intractable formulation, hence the use of model approximation is required. This computational study closely examines various approximation techniques in the context of multiparametric optimization and control with the use of key error metrics including: (i) open loop comparison of the high fidelity and approximate model, (ii) verification of step response profiles, and (iii) comparison of key features of the feasible space and objective function in the optimization formulation. Two systems are used as a basis for this study: a tank system utilized to highlight the main principles of this approach, and a Continuously Stirred Tank Reactor (CSTR) where the reaction mechanisms are manipulated to increase the model complexity.

Keywords: multiparametric programming, model reduction, model predictive control.

1. Introduction

Model based optimization for control, such as Model Predictive Control (MPC), has been gaining traction in the academic and industrial communities for more than 3 decades now (Camacho and Bordons, 2007). In recent years, more advanced models are being incorporated into these model predictive control frameworks (Santos et al, 2001). These direct formulations may typically result in an intractable, large scale, complex, non-convex optimization problem. Problems of this nature can be reduced to tractable forms via model approximation techniques (Diangelakis et al. 2017) that can then be solved offline explicitly using multiparametric programming (Bemporad et al., 2002).

Many techniques have been used for model approximation in Multiparametric Model Predictive Control (mpMPC), two common techniques include (piece-wise) linearization and system identification. Such model approximations are also at the heart of the PARameteric Optimization and Control (PAROC) framework for the derivation of these explicit/multiparametric controllers (Pistikopoulos et al., 2015). A key question that remains open within the PAROC framework is "*what constitutes a* <u>*suitable*</u> *approximate model for the derivation of explicit control strategies with multiparametric programming*?".

In this work, we present a computational study towards addressing this question. In particular, we study system identification (Ljung, 1998), and linearization. These model approximation techniques are widely used to develop linear discrete time state space models that can be incorporated into an MPC formulation. An additional approximation technique based on forward Euler discretization is also studied to compare against the aforementioned techniques. Key error criteria will be used to ascertain the effectiveness of each of the approximation techniques. These error criteria include: (i) open loop error analysis comparing the approximate model against the high fidelity model, (ii) step response profile analysis for each of the approximate models, (iii) comparison of the closed loop trajectory against the optimal trajectory determined from dynamic optimization in the gPROMS® environment, (iv) comparison of the objective values from the different mpMPC formulations and the optimal value determined in gPROMS®, and (v) comparison of the feasible space and objective function for the mpMPC formulations.

2. Methodology

The three approximation techniques used in the work are linearization, system identification, and a technique based on forward Euler discretization. Linearization is performed using first order Taylor Series approximation, where the linearization point is chosen to be at the defined set point of interest. In addition, system identification was performed using the MATLAB routine N4SID which is a subspace based approach to determine the state space matrices that best represent a set of outputs based on a given set of inputs.

The last approximation technique is based on Forward Euler discretization, which approximates the derivative information by taking a finite difference, instead of letting the limit approach zero, as seen in Eq.(1).

$$\frac{d\boldsymbol{x}}{d\boldsymbol{t}} = \boldsymbol{f}(\boldsymbol{x}) \Rightarrow \frac{\boldsymbol{\Delta x}}{\boldsymbol{\Delta t}} \approx \boldsymbol{f}(\boldsymbol{x_t}) \tag{1}$$

The benefit of this technique is that the derivate information is preserved through approximate discretization. As seen in Eq.(2), nonlinear state terms are treated as uncertain parameters, θ_t and ψ_t, to be used in an mpMPC formulation. In Eq.(2), the term $\psi_t u_t$ results in left hand-side uncertainty when formulated as an mpMPC problem. To avoid the challenges in solving a parametric programming problem with left hand-side uncertainty, this term can be grouped to form a new manipulated variable, as seen in Eq.(3). The new manipulated variables, $\tilde{u}$, will have varying bounds, which can be handled via multiparametric programming. However, grouping an uncertain parameter with a manipulated variable can only occur once for each manipulated variable.

$$\boldsymbol{x_{t+1}} = \boldsymbol{f}(\boldsymbol{x_t}) + \boldsymbol{g}(\boldsymbol{x_t})\boldsymbol{u_t} = \boldsymbol{\theta_t} + \boldsymbol{\psi_t u_t} \tag{2}$$

$$\boldsymbol{x_{t+1}} = \boldsymbol{\theta_t} + \boldsymbol{\tilde{u}_t} \tag{3}$$

The error criteria used in this work includes (i) root mean squared error deviation between the open loop profile for the high fidelity and approximate model, (ii) qualitative verification of the step response profiles of the approximate models, and (iii) comparison of the feasible space and objective function for the optimization formulations. Open loop analysis is performed using a random input profile on the high fidelity model and the approximate models developed. Step response profiles are verified based on how the real system is expected to perform. To compare feasible spaces of the optimization formulations, the volume of each feasible space is determined using Monte Carlo techniques, and to compare objective functions, the L^2 norm is used as seen in Eq.(4).

$$\|\boldsymbol{f}(\boldsymbol{x})\|_2 = \left(\int_{\boldsymbol{X}} |\boldsymbol{f}(\boldsymbol{x})|^2 \, \boldsymbol{dx}\right)^{\mathbf{0.5}} \tag{4}$$

3. Tank and Continuously Stirred Tank Reactor Examples

To demonstrate the criteria and approximation techniques used, a simplified tank system is examined. The tank has a fixed inlet flow and the flow out of the tank is manipulated via a valve on the exit of the tank. The control objective of the system is to maintain the level of the tank at a specified target. The system maintains a nonlinearity in the form of a square root, as seen in Eq.(5).

$$\frac{\boldsymbol{dh}}{\boldsymbol{dt}} = \frac{\boldsymbol{F}}{\boldsymbol{A}} - \boldsymbol{u}\sqrt{\boldsymbol{2gh}}\frac{\boldsymbol{A_{out}}}{\boldsymbol{A}} \tag{5}$$

The manipulated variable, u, maintains bounds between 0 and 1. The state of the system, h (m), must remain nonnegative. The parameters g (m/s^2), A (m^2), and A_{out} (m^2) are gravity, the area of the tank, and the outlet area of the tank respectively. The MPC formulation can be seen in Eq.(6).

$$\begin{aligned} &\min_{\boldsymbol{u}} \int_{\mathbf{0}}^{\boldsymbol{\tau}} \left(\left(\boldsymbol{x} - \boldsymbol{x_{ref}}\right)^{\boldsymbol{T}} \boldsymbol{Q}\left(\boldsymbol{x} - \boldsymbol{x_{ref}}\right)\right) \boldsymbol{dt} \\ &\boldsymbol{s.t.}\ \ \dot{\boldsymbol{x}} = \boldsymbol{Ax} + \boldsymbol{Bu}, \qquad \boldsymbol{x} \in \boldsymbol{X}, \boldsymbol{u} \in \boldsymbol{U} \end{aligned} \tag{6}$$

where Q is a cost matrix, x_{ref} is the set point of the system, x is the state of the system, and u is the input to the system. The MPC formulation can be discretized and converted to a multiparametric MPC where it is solved explicitly offline to determine the optimal control action as an affine function of the uncertain parameters, namely the initial state of the system and the set point.

As a second example, a single reaction, isothermal, and constant volume Continuously Stirred Tank Reactor (CSTR) is considered where the reaction rate complexity is increased. The reaction rate is either first order, second order, or third order. The CSTR has an adjustable flow rate of reactant into the reactor. Constant volume in the reactor is assumed and the reactor is considered to be isothermal. The control objective for this example problem is to maintain a specified reactant concentration level in the reactor while minimizing the use of the reactant flow.

$$\frac{\boldsymbol{dC_A}}{\boldsymbol{dt}} = \frac{\boldsymbol{F}}{\boldsymbol{V}}\left(\boldsymbol{C_{A_i}} - \boldsymbol{C_A}\right) - \boldsymbol{kC_A^{\alpha}} \tag{7}$$

$$\frac{\boldsymbol{dC_B}}{\boldsymbol{dt}} = \frac{\boldsymbol{F}}{\boldsymbol{V}}(-\boldsymbol{C_B}) + \boldsymbol{kC_A^{\alpha}} \tag{8}$$

The mass balance for the system can be described by Eq.(7) and Eq.(8), where the amount of reactant and product vary based on the inlet flow and the reaction mechanism. The manipulated flow into the reactor, F (m^3/s), is bounded between 0 and 1, and the states of the system, the reactant (C_A) and product (C_B) concentration (mol/m^3), are also bounded between 0 and 1. V (m^3) is the volume of the system, k is the rate constant of the system, C_{Ai} is the inlet reactant concentration, and the system order is α. The MPC formulation for this example problem, similar to Eq.(6), includes set point tracking on the reactant concentration, since there is a 1:1 correspondence between the reactant concentration and the product concentration, and a penalty on the usage of the reactant material, or a penalty on the input to the system.

4. Results and Discussion

Both examples were simulated and dynamically optimized using the gPROMS® software. The dynamic optimization was performed using Control Vector Parameterization which discretizes the manipulated variable over a control interval, and over each interval the manipulated variable is assumed to follow a simple function. The optimal trajectory determined from gPROMS® is considered as the optimal trajectory and is compared against the mpMPC closed loop trajectories. The objective function used in the mpMPC formulation is the same in all formulations. For the mpMPC formulations, the output and control horizon is 3 and 2 respectively for the tank example and 5 and 2 respectively for the CSTR example.

Figure 1a shows the open loop response of the approximate models and the high fidelity model for the tank example, where the legend shows the root mean squared error. The open loop performance of system identification performs the worst out of the approximation techniques, and linearization performs the best. Figure 1b is a comparison of the step response profiles. All of the step response profiles show a decrease in the output for an increase in the input, which is consistent with how the system would react. The approximate model resulting from forward Euler discretization is a straight line because the state space representation is critically stable. Figure 2 shows trajectories from using different approximate models and control strategies, and the corresponding output of the system. The optimal trajectories are determined from the mpMPC formulation, a dynamically optimized PI controller, and open loop dynamic optimization on the full process model in gPROMS®. Table 1 shows a comparison of the objective function costs, volume of the feasible space, and distance between objective functions. From Table 1, based on the objective function costs, linearization has the most comparable performance to the open loop dynamic optimization results. This can be attributed to linearization performing well around the linearization point, which was chosen as the set point. Forward Euler has a similar cost and an objective function that more closely matches the 'real' objective function. System identification performs the worst, except it has a feasible space volume that is closer to the actual the feasible space volume.

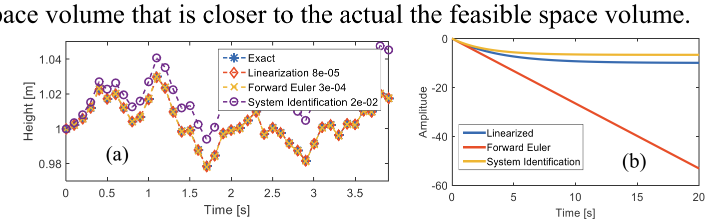

Figure 1. (a) Open loop comparison of output via root mean squared error (b) Step response profiles of the approximate models for the tank example

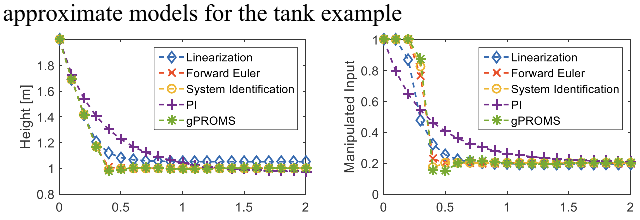

Figure 2. Closed loop performance comparison for the various controllers and open loop dynamic optimization for the tank example

Table 1. Quantitative results of different error criteria

	Linearization	System Ident	Forward Euler	Exact
Optimal Trajectory Cost (Tank)	1.1264	1.12738	1.12723	1.1261
Feasible Space Volume (Tank)	98	98.3	94.9	100
Objective Function L^2 (Tank)	5.19	13.42	0.1497	0
Optimal Trajectory Cost (CSTR),α=1	0.139	0.140	0.140	0.135
Feasible Space Volume (CSTR), α=1	0.47	0.44	0.26	1
Objective Function L^2 (CSTR), α=1	0.54	0.42	3.1604	0
Optimal Trajectory Cost (CSTR),α=2	0.112	0.113	0.112	0.110
Feasible Space Volume (CSTR), α=2	0.41	0.38	0.19	1
Objective Function L^2 (CSTR), α=2	0.67	1.54	4.22	0
Optimal Trajectory Cost (CSTR),α=3	0.174	0.181	0.174	0.173
Feasible Space Volume (CSTR), α=3	0.36	0.43	.22	1
Objective Function L^2 (CSTR), α=3	0.84	1.25	4.22	0

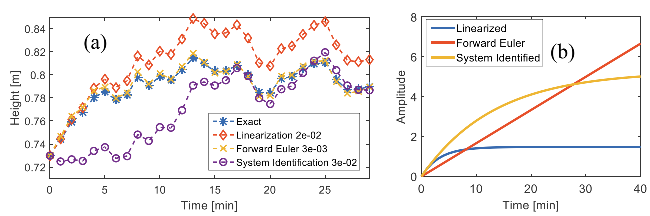

Figure 3. (a) Open loop comparison of output via root mean squared error (b) Step response profiles of the approximate models for the CSTR example

The open loop performance and step responses for the CSTR are only compared for an α value of 3. As seen in Figure 3a, the open loop performance of system identification performs the worst out of the approximation techniques. Figure 3b is a comparison of the step response profiles. All of the step responses show an increase in the output concentration for an increase in the input, as expected for this system. Forward Euler approximation has a straight line due because its state space model is critically stable. Figure 4 shows optimal trajectories from using different approximate models and techniques, and the corresponding output of the system. The optimal trajectories are determined from the mpMPC formulation, a dynamically optimized PI controller, and open loop dynamic optimization on the full process model. Comparison of the objective function costs, volume of the feasible space, and distance between objective functions can be seen in Table 1. For all of the different values of α, linearization performs the best, while maintaining a feasible space and objective function most similar to the real system. Because the system has a set point that matches the linearization point the linearized state space model can accurately represent the system in this region. Forward Euler performs well for all α even though it has a feasible space that is smaller than both the system identification and linearization feasible spaces. Its objective function distance is also farther away than the objective functions for both linearization and system identification. The feasible space being small is not enough on its own to categorize poor performance and the distance in objective functions is not large enough to cause performance issues either.

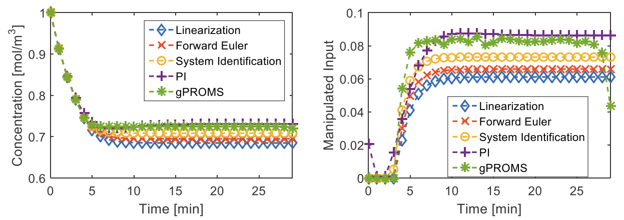

Figure 4. Closed loop performance comparison for the various controllers and open loop dynamic optimization for the CSTR example

5. Conclusions

Various model approximation techniques have been utilized to develop multiparametric model predictive controllers. These approximate models and resulting optimization formulations were assessed using various error criteria. For the example problems presented, and criteria used, the linearization technique provided an optimal trajectory that was closest to the 'desired' trajectory using dynamic optimization in gPROMS®. Future work is to apply these concepts on a system of significantly increased complexity and further development on the concepts of feasible space volume and distance between objective functions.

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