Linear MPC based on data-driven Artificial Neural Networks for large-scale nonlinear distributed parameter systems

Weiguo Xie, Ioannis Bonis, Constantinos Theodoropoulos*

School of Chemical Engineering and Analytical Science, University of Manchester, Sackville Street, Manchester M13 9PL, UK.

Abstract

Process controller synthesis with detailed models is a challenging task, which may lead to many advantageous closed-loop features. Model reduction such as Proper Orthogonal Decomposition (POD) and (adaptive) linearization can be applied to tackle with the arising problems, whereas process data can be directly used to build accurate models via training of artificial neural networks (ANN). In this contribution, we present two methodologies we have recently developed, which combine ANN with POD, for use in the context of MPC: the process at hand is represented as a sum of products of time-varying coefficients (computed with ANN) with the POD basis functions computed from plant “snapshots”. The resulting accurate model can be used in NMPC, or trajectory piecewise linearization along a reference path can be applied on the ANN, yielding a series of linear models, suitable for linear MPC.

Keywords: Model predictive control, proper orthogonal decomposition, neural network training, reduced order NMPC, model reduction for (non-)linear predictive control.

1. Introduction

The use of detailed models in process control has a number of advantages, such as flexibility in operating conditions, relatively small plant/model discrepancy and reliable compliance with constraints. For most processes such detailed models exhibit nonlinearity and often high dimensionality, which is especially the case for distributed parameter systems as their solution follows from spatial discretization. The first issue can be coped with linearization (at a stationary point or along a trajectory) and the second with model reduction techniques such as POD. Additional issues arise if there is uncertainty in process parameters or even the governing equations. ANN can be used to simulate the plant at hand, requiring only a set of process data for training. The algorithms presented in this work rely on the provision of an ensemble of process “snapshots” (Atwell and King, 2004), which can be used to obtain an empirical set of eigenfunctions spanning the feasible state space. The state vector at any time instance can be approximated as a linear combination of these eigenfunctions. The coefficients in this formulation are time-varying and are typically computed from a Galerkin projection on the governing equations, although other approaches have been followed (cf. Aggelogiannaki and Sarimveis, 2008; García et al., 2007). Here, the time coefficients are computed from ANN, suitably trained using process data. Since in POD only the most important eigenfunctions are used, the dimension of the time coefficients, hence the ANN is typically small, allowing incorporation to nonlinear MPC, leading to the

* Corresponding author, e-mail: k.theodoropoulos@manchester.ac.uk
first of the algorithms presented in this contribution. Its main feature is the explicit formulation of the constraints in terms of time coefficients, resulting in efficient schemes. Conversely, nonlinear controllers are avoided in practice. We therefore consider linearising the ANN in an error-controlled fashion following the reference trajectory piecewise linearization paradigm (Rewienski and White, 2003). This leads to a sequence of linear models obtained using the ANN (thus solely process data). This sequence can be employed in a linear MPC strategy, which bears resemblance to the multi-model/gain-scheduled model predictive control (Özkan et al., 2003). This work exploits the time-space separation, feature which is often utilized in the case of DPS (Li and Qi, 2010). Recently, we have presented a strategy for linear MPC using POD models and temporal reference trajectory linearization (Xie et al., 2011). Here we extend this work for systems, where a Galerkin projection is strenuous or problematic.

2. Nonlinear Model Reduction

2.1. Proper Orthogonal Decomposition

POD is a powerful model reduction technique, which results in the states $x(z,t)$ of the system being expressed as the product of time-invariant, space-varying basis functions $\varphi(z)$ and time-varying coefficients $a(t)$. The eigenfunctions $\varphi(z)$ can be computed from an ensemble of dynamical process data (“snapshots”) for a range of parameters, appropriately assorted in a 2-point correlation matrix. Thus:

$$x(z,t) = \sum_{i=1}^{m} a_i(t) \varphi_i(z) + \bar{x}(z)$$

where $\bar{x}(z)$ is the average state variable vector of the snapshots used. The number of modes, $m$, used is empirically defined, in such a way that most of the “energy” of the system is captured, i.e. the reduced model sufficiently approximates the full one. Eq. (1) illustrates the time-space separation nature of the reduction strategy. Moreover, since the space-varying terms are computed from the (constant) snapshots, the only variable in Eq. (1) is time (1D relation).

2.2. Computing the time coefficients of POD with Neural Networks

A conventional way of computing POD time coefficients is by nonlinear Galerkin projection of the governing equations on the POD basis functions, from which relations for $a(t)$ can be obtained. However, in cases that these equations are uncertain or even unknown, the procedure outlined may prove problematic. In this work, ANNs are used for computing the time coefficients. An Elman neural network (Cheng et al., 2002) is employed, the training of which follows from a nonlinear least squares optimization problem. If a single ANN is unable to capture the dynamic behavior of $a(t)$, a sequence of ANNs can be used, each one of which is valid for a certain region in the time domain.

2.3. Adaptive trajectory piecewise linearization of ANN

The ANN is based on input/output data, but does provide an analytical expression for $a(t)$. These relations can be linearized adaptively on a reference trajectory, resulting in a sequence of linear models, each being valid for a range of times. The procedure outlined here follows the paradigm presented in (Xie et al., 2011). The purpose is to approximate $a(t)$ with piecewise linear interpolations $L_j(t) = b_j + c_j$. Considering partitioning the time domain in regions of uniform length, the number of regions that needs to be created to allow approximation with a given tolerance $\delta$, is (Van Loan, 1997):

$$n_{pw_l} \geq 1 + (t_{\text{fin}} - t_{\text{init}}) \sqrt{M_2/(8\delta)}$$

Where \( M_2 \) is an estimate of the norm of the 2nd derivative of \( \alpha(t) \). Hence we have the partition:

\[
t_{\text{init}} = t_1 < t_2 < \cdots < t_n = t_{\text{fin}}, \quad \text{with } t_i = t_{\text{init}} + (i - 1)(t_{\text{fin}} - t_{\text{init}})/(n_{\text{tpwl}} - 1).
\]

The procedure outlined so far in this section is referred to as **static TPWL** and may lead to conservative estimates for \( n_{\text{tpwl}} \). We can refine the partition (3) following an iterative **adaptive TPWL** procedure, which considers merging neighboring regions. A candidate interval \([t_L, t_R]\) is deemed acceptable, if:

\[
\left| a_j \left( \frac{t_L + t_R}{2} \right) - a_j \left( t_L \right) + a_j \left( t_R \right) \right| \leq \delta \quad \text{and} \quad 0 < t_R - t_L \leq h_{\text{min}} \quad (4)
\]

where \( h_{\text{min}} \) is a heuristically chosen parameter and \( a(t) \) is given by the ANN. The new number of TWPL horizons, \( n_{\text{tpwl}} \), is the minimum number of subintervals satisfying Eq. (4) defining a partition of \( t \). For a partition \( j \): \( a(t) = L_j(t) = b_j t + c_j \), for \( t \in [t_j, t_{j+1}) \).

### 3. The MPC formulations

**3.1. The POD-ANN-NMPC controller**

The ANN for the time coefficients trained as described in Section 2.2, can be combined with the POD basis functions to give an estimation of the states for any given time, subject to initial conditions. This nonlinear model can be used to formulate a Nonlinear Model Predictive Controller, for the computation of a sequence of future control actions:

\[
\min_{DU} J = \left\| \sum_{k=1}^{n_{\text{tpwl}}} a_{k,1}(t)\sigma(z) + T_{\text{ref}}(t) - T_{a}(t) \right\|_Q + \left\| DU \right\|_R
\]

s.t. \( a_{k,1}(t) = LW_{3,2} \cdot \alpha_1(t) + b_1 \)

\[
a_1(t) = \tanh(IW_{1,3} \cdot U + LW_{1,3} \cdot a_1(t - 1) + b_1)
\]

\[
a_2(t) = \tanh(LW_{2,3} \cdot a_1(t) + LW_{2,2} \cdot a_2(t - 1) + b_2)
\]

where \( LW, IW \), and \( b \) are obtained from the network training, and \( a_j(t), a_2(t) \) are internal output parameters of the first two ANN layers. The main feature of the optimal control problem (5) is that the objective function and the (equality and any inequality) constraints are written explicitly in terms of the ANN outputs. There are many efficient ways of solving (5) (Biegler, 2000); here we follow a sequential approach.

**3.2. The POD-ANN-TPWL-MPC controller**

Although the optimization problem (5) is reduced, and there exist efficient methods for its solution, it is still nonlinear and that may be deemed as a disadvantage, due to its complexity and computational requirements. We can apply the procedure of Section 2.3 to obtain a sequence of linear models, which approximate the system sufficiently well (i.e. abiding by a given tolerance) that can be used for linear MPC. At the time-points where the linear interpolation point changes, a linear MPC controller needs to be reformulated based on the governing linear model. In this case, the future sequence of control actions is computed as a result from a quadratic optimization problem:

\[
\min_{DU} J = \left\| \sum_{k=1}^{n_{\text{tpwl}}} (b_j t + c_j)\sigma(z) + T_{\text{ref}}(t) - T_{a}(t) \right\|_Q + \left\| DU \right\|_R \quad k = 1, \ldots, n_{\text{tpwl}}
\]

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4. Case study: control of a tubular reactor with recycle

To illustrate the performance of the controllers designed following above concepts, we have applied them for the control of a tubular reactor with recycle (Fig.1). The PDE-based model of the reactor and the parameter values chosen can be found elsewhere (Xie et al., 2011). The same procedure can be applied even in the absence of such an explicit model, using model/process data. The system is stable for \( r=0 \), but exhibits sustained oscillations for \( r=0.5 \). Fig.2 depicts the time profiles for temperature at the centre and exit of the reactor obtained using the full (PDE) model and the reduced POD-ANN one. We consider 8 cooling zones in the reactor jacket, the temperature of which can be controlled independently and comprise the controlled variables. The objective of the controllers is to stabilize the system with \( r=0.5 \). This is handled as a setpoint tracking problem: both temperature and concentration at the reactor exit are required to follow a time varying setpoint signal obtained from open-loop system simulations for \( r=0 \). Using the POD-ANN-NMPC formulation, we achieve the closed loop behavior of Fig.3a. Corresponding control actions are presented in Fig.3b. The setpoint tracking capability of the controller is satisfactory. The noise in the inputs computed can be decreased by filtering the ANN, or by implementing suitable constraints in the NMPC problem; both directions will be explored in future work. We have additionally considered more complicated control problems based on this case study, involving unstable setpoint signals and inequality constraints; the corresponding results will be presented in an extended publication. We have also obtained a linear controller based on the POD-ANN-TPWL-MPC scheme of Section 3.2. The closed-loop behavior is illustrated in Fig.4a and the corresponding inputs in Fig.4b. The response in this case is worse than the one obtained with the nonlinear controller. Noise is due to the linearisation of the ANN, the intrinsic noise of which results in large gradients. Filtering the ANN before the TPWL step can enhance performance.

5. Conclusions

We have presented two MPC methodologies, which employ accurate low-order models based on Proper Orthogonal Decomposition in conjunction with Neural Networks. Direct utilization of such models in MPC leads to nonlinear control schemes. If TPWL is applied along a reference trajectory, a controller synthesis framework following the (linear) multi model predictive control paradigm is obtained. The second approach has been shown to exhibit slightly worse closed-loop behavior, but increased efficiency and
Figure 3: Stabilisation with the POD-ANN-NMPC scheme (a) and corresponding inputs (b).

Figure 4: Stabilisation with the POD-ANN-TPWL-MPC scheme (a), corresponding inputs (b).

decreased complexity. Both formulations can be used for the challenging setpoint tracking control problem, which is a nontrivial feature for ANN-based models.

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