

# Multimodel Decomposition of Nonlinear Dynamics Using Fuzzy Classification and Gap Metric Analysis

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**Abstract:** Identification of accurate nonlinear models is central to the success of the nonlinear model based schemes. Approximation of the nonlinear system dynamics in a multiple linear model framework has been well addressed in the literature. However, such multimodel decomposition can result in unstable local models. Additionally, the number of local models to be selected for the nonlinear identification is critically dependant on the partitioning approach. This paper proposes a novel gap metric based fuzzy decomposition of nonlinear dynamics using multiple, locally linear models. Such a decomposition is shown to result in a stable and parsimonious model set which can be deployed for online control. A simulation case study involving nonlinear polystyrene reactor, is presented to illustrate the proposed approach.

*Keywords:* NLID, Gap Metric, Fuzzy Classification

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## 1. INTRODUCTION

Nonlinear process control methodologies are typically deployed for flexible and improved productivity in polymer, chemical, paper and pulp industries. These processes often require product grade transitions to fulfill customer needs and to seek benefits of market dynamics. Due to requirement of such flexible mode of operation, these processes need to be transitioned and regulated over a broad range of operating conditions. The process dynamics change significantly during such transitions and therefore, the underlying dynamic models used in the controller need to be updated. These dynamic models represent the dynamic relationship between the manipulated variables (MVs) that are frequently updated by the controller to regulate the controlled variables (CVs), in the presence of disturbance variables (DVs). Due to such a wide range of operating conditions and frequent grade transitions, the underlying process dynamics become nonlinear in nature. This nonlinear dynamics can be captured by employing a single monolithic nonlinear model or by dividing the nonlinear dynamics into multiple linear or simpler nonlinear models. Typically, the first principle based models fall under the first category (single monolithic model) and are very complex, difficult and expensive to build. The use of such a complex nonlinear model in the NMPC can lead to numerical and computational issues. In some cases, the solution of the optimisation problem can become infeasible or non optimal. An alternate attractive approach that can solve such problems is to decompose the nonlinear dynamics into multiple linear models and then switch smoothly among the models based on the current state of the process. In such a case, the NMPC optimisation problem based on linearised models becomes better structured and can be

solved in quick time. Due to these benefits, the multiple model based nonlinear identification strategy looks more promising and practical.

One approach to multi model decomposition of non linear dynamics has been proposed by Wojsznis et al. (2005). The approach performs interpolation between local model parameters based on some heuristics and model validity measures. However, the heuristic based approach is not good enough for a wide variety of applications. The method also assumes homogeneity of the local models and linear interpolation of the model parameters. An alternate approach is proposed by Narendra and Balakrishnan (1997). However, this approach assumes availability of knowledge of various operating regions, their ranges and their centres. Skarmeta et al. (1999) have proposed a fuzzy classification based multi model decomposition approach. However, this approach does not consider stability analysis in selecting the optimal number of local models. Galan et al. (2003), have applied the stability analysis in selecting the optimal number of local models in their paper. However, in this approach the local models are not obtained via data based modeling but are developed using linearization of first principle based model. Venkat et al. (2003) have proposed a strategy for building multiple local linear/simpler nonlinear models based on an analysis of the dynamic input-output data obtained by plant perturbation. Gugaliya et al. (2005) have proposed a Fuzzy-CART based multimodel development strategy based on dynamic plant data classification. In most of the above strategies, the focus on the development of a smooth switching strategy has not been considered for the selected local models. Additionally, the closed loop stability considerations are missing while developing this set of local models.

Specifically, for the multiple models based identification approach, the model identification procedure has to address many issues, primary amongst them are i) Selection of number of local models, ii) Development of the local models, iii) Switching strategy between the models when the models are deployed online and iv) Closed loop stability when the model switching is done. This latter aspect of closed loop stability is very important issue in determining the controller performance when these set of models are deployed for online control.

This paper explicitly uses stability considerations in partitioning/decomposition of the nonlinearity. Since the local models would be used in closed loop control, it is of high importance to ensure that the models along with the local controller provide for closed loop stability. This paper proposes the use of the gap metric which measures the relative stability of dynamic models from a closed loop stability viewpoint. This metric is therefore explicitly suited for use as measure of overall closed loop stability in a multimodel context and is therefore exploited in this paper. Earlier approaches towards decomposition of nonlinearity ignored this stability aspect and therefore are relatively prone to yield models that could provide a cause of instability. This paper also contributes in combining the fuzzy-classification based multimodel decomposition of nonlinear dynamics method with the gap metric based model set reduction method. Together, this combination provides a smooth switching strategy and ensures a parsimonious and robust model set to be deployed for online control.

This paper is organised as follows : Section 2 explains in detail the fuzzy classification based multiple model approach towards nonlinear identification. Section 3 explains the gap metric based model set reduction step. Section 4 illustrates the polystyrene case study with representative results. Section 4 summarises the work and provides pointers to the future work.

## 2. FUZZY CLASSIFICATION BASED LOCAL MODEL DEVELOPMENT

The central principle of most fuzzy based partitioning schemes is to adopt a divide and conquer strategy, i.e. partition the complex nonlinear dynamics into simpler local models. Towards this objective the nonlinear processes are first perturbed in all the possible operating regimes and the corresponding dynamic data is then utilised to develop multiple local linear or simpler nonlinear models. The overall architecture of the approach is represented in Figure 1 which clearly depicts the various steps involved in the proposed approach.

In the sequel, each of the blocks in the above architecture will be briefly elaborated upon.

**Excitation signal design:** The nonlinear process needs to be perturbed over a broad range so that the nonlinear dynamics are excited across all the operating regimes of the process. The accuracy of these identified dynamics strongly depend on the quality of the excitation signals employed for perturbing the process. The identification exercise is a time consuming and expensive step and therefore these excitation signals need to be carefully designed. For nonlinear identification, the excitation signals need to have

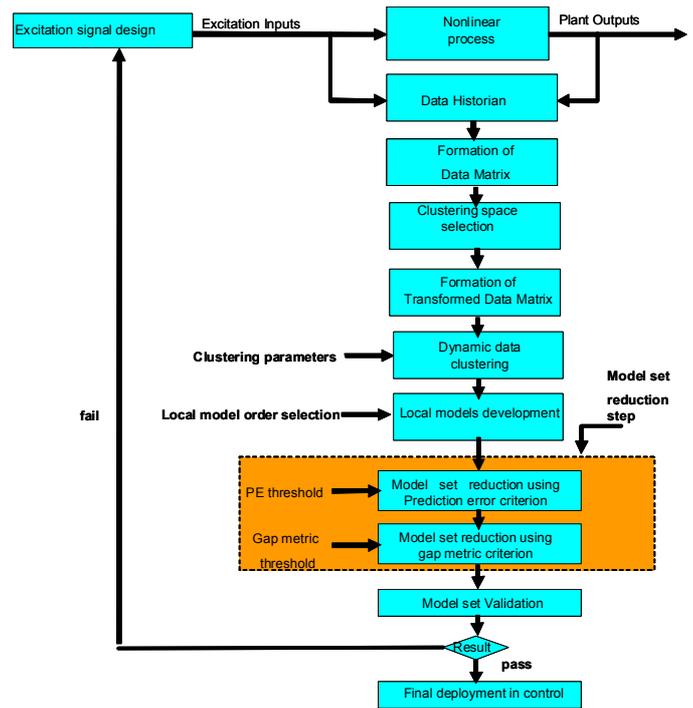


Fig. 1. Architecture of the Proposed Approach

a spectra of amplitudes (multilevel signals) as well to capture the process nonlinearity. Typically staircase signals or multi-sine signals are known to have this feature. Moreover, the PRBS or GBS signals can be modified to have multiple levels (Godfrey, 1993). Any of these signals can be used for nonlinear process identification. The amplitude band for these signals is decided by the range of dynamics that needs to be identified and the dominant process gains. The frequency band of these signals is decided by the range of time constants of the process over the intended range of process operation. It is recommended to perturb multiple MVs simultaneously to reduce the identification test time as well as to capture plant directionalities. However, the process safety considerations must be respected while perturbing multiple MVs simultaneously. The guidelines for the signal design can be refined and corrected by model validation tests.

**Data Cleaning:** The plant data comprising the MV-DV-CV variables is subjected to data cleaning operation. The data cleaning operation typically involves outlier removal, data pre-filtering (for suppressing process noise) and data scaling. The cleaned plant data is then partitioned into two data sets namely training data set and validation data set. The training data set is used for local models development and the validation data set is used for testing the validity of the identified models. Typically, 60% of data points can be used for model development and 40% of data points can be used for model validation. This split ratio can differ from case to case.

**Dynamic Clustering Space (DCS) selection:** The cleaned process data needs to be partitioned to generate the multiple linear models. Such partitioning has to be carried out in an appropriate data space comprising of different lags of the MVS, DVS and CVs, so that the dynamic behaviour is captured properly. Such data space

is defined as dynamic clustering space (DCS). The choice of DCS is dependent on presence of delays and nature of the dynamics of the local regions. Various DCS selection strategies have been explained in detail by Venkat et al. (2003).

**Dynamic data clustering:** The DCS selected by the earlier step is used to modify the MV-DV-CV data, so that each row of the new data matrix represents a point in the clustering space. The modified dynamic data is subjected to fuzzy clustering algorithm. The objective of the algorithm is to identify the local regions wherein a linear/simple nonlinear model can be fitted. This algorithm enables the division of the complex nonlinear spaces into elementary subspaces. This algorithm also ensures overlap of the subspaces for representing the nonlinear behaviour in transition regions. The data points having similar dynamic relationship are clustered together. There are well known fuzzy clustering algorithms, namely Gustafson-Kessel algorithm and Fuzzy C means clustering (FCM). However, these algorithms have been shown to potentially yield suboptimal solution. Therefore, it is desirable that the fuzzy clustering is to be carried out in a Monte Carlo framework. Monte Carlo simulations can be generated by running this algorithm using different initial guesses of the initial membership matrix, due to which the chances of locating the globally optimal partition can be improved. It should be noted that the number of clusters to be identified ( $c$ ) has to be provided to the fuzzy clustering algorithm. However, in practical situations, this information is not available a priori. In this paper, the fuzzy clustering algorithm is initiated with large number of clusters (roughly  $\frac{1}{20}^{\text{th}}$  of the data size) and then the cluster merging is done at a later stage based on the criteria of parsimony and stability.

**Local model development:** The aforesaid clustering algorithms provides  $c$  clusters along with the corresponding partition matrix for each cluster. In this step the local models are developed within each cluster. Towards this model building step, data points with degree of membership value greater than a fixed threshold are considered for each cluster. This enables filtering out of the noisy data points and thereby considering those data points which are relevant to the cluster. Model order selection has to be judiciously carried out to develop good quality models. This can be done using AIC (Akaike Information Criterion) or any similar criterion. Otherwise, a series of model orders can be chosen and the local model that provides the best prediction capabilities can be chosen as the local model order. The parameters of the local model can be identified by the least squares method.

**Compositions of local models to obtain aggregated output:** The predictions out of the  $c$  locally linear models obtained in the earlier step need to be suitably aggregated so as to predict the actual output of the system. When the system is operating in the region corresponding to a cluster, the model corresponding to this cluster is utilised for prediction. When the system is in transition phase, then a suitable combination of the local model predictions, is utilised to predict the system dynamics. These local model predictions are combined based on the degree of

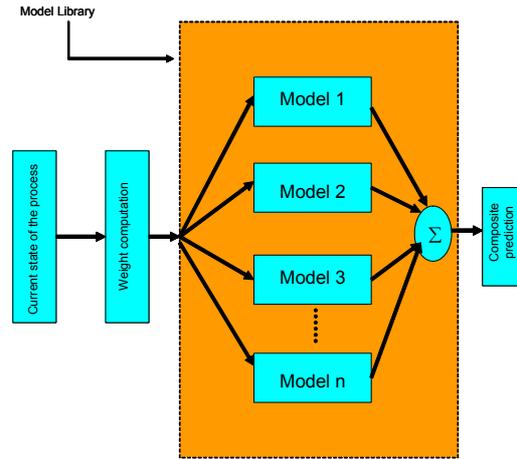


Fig. 2. Composite Prediction Mechanism

membership of the current state to each of the individual cluster.

Figure 2 depicts the calculation of the aggregated output.

### 3. GAP METRIC BASED MODEL REDUCTION

As discussed earlier, the fuzzy clustering is done with a large number of clusters so that the prediction error is minimal. However, the selection of the actual number of clusters has to be done judiciously. If a large number of clusters are selected, the composite prediction model will capture the process nonlinear behaviour very well (low prediction error). However, such a composite model comprising large number of local models, is difficult to deploy for controller design. The maintenance of the controller also becomes prohibitively complex.

Therefore, it is necessary to reduce the number of models so that the underlying controller becomes simple. For the case of large number of models, the models so identified are also relatively similar to each other, and there is scope for merging of some of the models without significantly affecting the prediction quality of the composite models. However, merging of the clusters has to be done while keeping in view the intended end use of the models i.e. closed loop control. Therefore, the decision step of selection of optimal number of clusters has to simultaneously consider both closed loop stability issues and prediction error based model quality issues. Towards the closed loop stability issues, gap metric based approach is proposed in this paper. The Gap metric (Georgiou, 1988) provides a measure to calculate the distance between the two dynamic systems from a closed loop stability view point. Typically the gap metric for two SISO dynamic models  $P_1$  and  $P_2$  can be calculated as :

$$\delta(P_1, P_2) = \sup_{\omega} \frac{|P_1(j\omega) - P_2(j\omega)|}{\sqrt{1 + |P_1(j\omega)|^2} \sqrt{1 + |P_2(j\omega)|^2}} \quad (1)$$

where  $0 \leq \delta \leq 1$ ,  $P_1(j\omega)$  and  $P_2(j\omega)$  represent the frequency responses of the system  $P_1$  and  $P_2$  respectively. A value of  $\delta$  close to 0 represents that the two models are similar and can be merged whereas value of  $\delta$  close to 1 indicates that the two dynamic models behave differently

when placed in a control loop. Merging of such models (having  $\delta$  close to 1) can result in closed loop instability. Since model discrimination is enabled by the gap metric criterion, from the closed loop stability perspective, it is therefore meaningful to use this criterion while assessing the number of local models. Here we propose the model set reduction using gap metric analysis for data cluster merging be applied after the model set reduction using prediction error. Therefore, at the end of these two steps, it is expected that a set of models satisfying the prediction error and gap metric criteria will be obtained.

*Gap metric analysis for cluster merging:* In this paper, the fuzzy clustering algorithm is initiated with large number of clusters (roughly  $\frac{1}{20}$ th of the data size). The fuzzy classification algorithm then partitions the dynamic data into multiple clusters. The data in each cluster is then used to develop the local model. Model order selection has to be judiciously carried out to develop good quality models. This can be done using AIC (Akaike Information Criterion) or any similar criterion. Otherwise, a series of model orders can be chosen and the local model providing best prediction capabilities can be chosen as the local model order. The parameters of the local model can be identified by least squares method. The gap metric analysis is performed on the series of local models to compute the gap matrix (G) of dimension  $c \times c$ , wherein  $G_{i,j}$  entry represents gap metric value between model  $i$  and  $j$  respectively. The diagonal entries in the G matrix will be zeros and G matrix will be symmetrical in nature as  $G_{i,j} = G_{j,i}$ .

Once the G matrix is computed, the matrix is scanned for models which can be merged. A threshold value of  $\delta$  ( $\delta_{threshold}$ ) is chosen based on the stability sensitivity of the nonlinear process under consideration. Typically the threshold value of  $\delta_{threshold}$  varies between 0 to 0.5 where threshold value 0 indicates no model merging case and progressively increasing values towards 0.5 indicates relatively relaxed stability norm consideration for model merging. Based on the value of  $\delta_{threshold}$ , the set of local models to be merged are identified. The local data in the corresponding clusters are merged and the model parameter identification is performed on the merged data set to get a new local model. The new local model replaces the merged models and the membership value of a data point to the the new local model is the sum of membership values of the data point to the merged models. Using the updated membership function, the composite prediction of the merged model set is computed on a validation data set.

*Prediction error analysis for cluster merging:* As discussed in the above step, the composite prediction error of the reduced set of the models is computed on the validation data set. The composite prediction error of the full model set (prior to model reduction step) is also computed on the validation data set. The difference between the two prediction errors is computed and compared with the threshold for prediction error analysis. The criterion on prediction error threshold can be chosen in terms of certain percentage deviation of prediction error from the full model set case. If the increase in prediction error due to the model reduction step is below the threshold value, the model merging is accepted. Otherwise, the threshold

on the gap metric analysis ( $\delta$ ) is tightened and the model merging is iterated. This procedure is iterated till the criteria based on gap metric threshold and prediction error threshold are satisfied simultaneously. In the next Section we validate the proposed approach on a nonlinear simulation case study.

#### 4. RESULTS AND DISCUSSION

The nonlinear process used for this study is the continuously stirred tank reactor (CSTR) wherein polymerization of styrene to polystyrene takes place (Tatiraju & Soroush,1999). The simplified process flow sheet is shown in Figure 3. The process model for the polymerization of styrene in a jacketed continuous stirred tank reactor (CSTR) involves reaction kinetics, a material balance and an energy balance. The CSTR has three feed streams-pure styrene monomer, azobisisobutyronitrile (AIBN) initiator dissolved in benzene and pure benzene(solvent). The cooling jacket uses water as the cooling fluid to remove heat generated by the exothermic polymerization. There is one exit stream containing polymer, un-reacted monomer, initiator and solvent. The model for the polymerization includes following set of Equations,

$$\frac{d[I]}{dt} = \frac{(Q_i[I_f] - Q_t[I])}{V} - k_d[I] \quad (2)$$

$$\frac{d[M]}{dt} = \frac{(Q_M[M_t] - Q_t[M])}{V} - k_p[M][P] \quad (3)$$

$$\frac{d[T]}{dt} = \frac{Q_t(T_f - T)}{V} + \frac{-\Delta H_r}{\rho C_p} k_p[M][P] - \frac{hA}{\rho C_p V} (T - T_c) \quad (4)$$

$$\frac{d[T_c]}{dt} = \frac{Q_c(T_{cf} - T_c)}{V_c} + \frac{hA}{\rho_c C_{pc} V_c} (T - T_c) \quad (5)$$

$$P = \left[ \frac{2fk_d[I]}{k_t} \right]^{1/2} \quad (6)$$

The CSTR case study is shown to be highly nonlinear and complex from control perspective. The various constants for the process model can be found in Hidalgo and Brosilow (1990). There are two manipulated variables (MVs) namely the initiator flow rate and coolant flow rate and two controlled variables (CVs) namely the reactor temperature and monomer conversion. In order to perform identification using the approach proposed in this paper, CSTR is perturbed with the multilevel excitation signals. The corresponding process data is subjected to fuzzy classification as depicted in Figure 1. The DCS is selected as past two lags of inputs and one lag of output. The fuzzy clustering algorithm is initiated with 8 clusters and the dynamic data in each cluster is modelled using ARX structure. The results of the composite predictions using these models are shown in Figure 4. The gap metric matrix G for these 8 models is computed and is depicted in Equation 7,

$$G = \begin{bmatrix} 0 & 0.8 & 0.68 & 0.62 & 0.59 & 0.38 & 0.25 & 0.29 \\ 0.8 & 0 & 0.39 & 0.09 & 0.55 & 0.92 & 0.79 & 0.61 \\ 0.68 & 0.39 & 0 & 0.35 & 0.51 & 0.61 & 0.55 & 0.75 \\ 0.62 & 0.09 & 0.35 & 0 & 0.65 & 0.66 & 0.48 & 0.85 \\ 0.59 & 0.55 & 0.51 & 0.65 & 0 & 0.72 & 0.42 & 0.76 \\ 0.38 & 0.92 & 0.61 & 0.66 & 0.72 & 0 & 0.35 & 0.19 \\ 0.25 & 0.79 & 0.55 & 0.48 & 0.42 & 0.35 & 0 & 0.21 \\ 0.29 & 0.61 & 0.75 & 0.85 & 0.76 & 0.19 & 0.21 & 0 \end{bmatrix} \quad (7)$$

- Q Quantity
- A Heat Transfer area of CSTR
- $C_p$  Mean heat capacity of reactor fluid
- $C_{pc}$  Heat capacity of cooling jacket fluid
- f Initiator efficiency
- h Overall heat transfer coefficient
- I Concentration of initiator in reactor
- $I_f$  Concentration of initiator in feed
- $k_d$   $A_d \cdot \text{Exp}(-E_d/T) \text{Sec}^{-1}$
- $k_p$   $A_p \cdot \text{Exp}(-E_p/T) \text{mol}^{-1} \text{Sec}^{-1}$
- $k_t$   $A_t \cdot \text{Exp}(-E_t/T) \text{mol}^{-1} \text{Sec}^{-1}$
- M Monomer concentration in reactor
- $M_f$  Monomer concentration in feed
- $Q_i$  Flow rate of initiator stream
- $Q_c$  Flow rate of cooling jacket fluid
- $Q_m$  Flow rate of monomer stream
- $Q_t$  Flow rate of exit stream ( $Q_i + Q_s + Q_m$ )
- t Time
- T Temperature of Reactor
- $T_c$  Mixing cup of cooling jacket fluid
- $T_{cf}$  Inlet temperature of cooling jacket fluid
- $T_f$  Temperature of reactor feed
- V Reactor volume
- $-\Delta H_r$  Heat of polymerisation reaction
- $\rho$  Mean density of reactor fluid
- $\rho_C$  Density of cooling jacket fluid

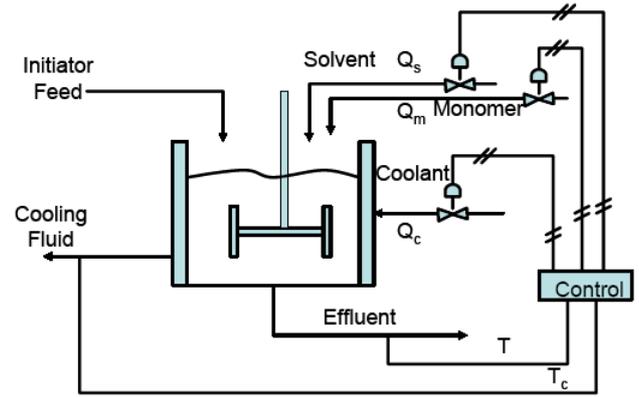


Fig. 3. Polystyrene Case Study

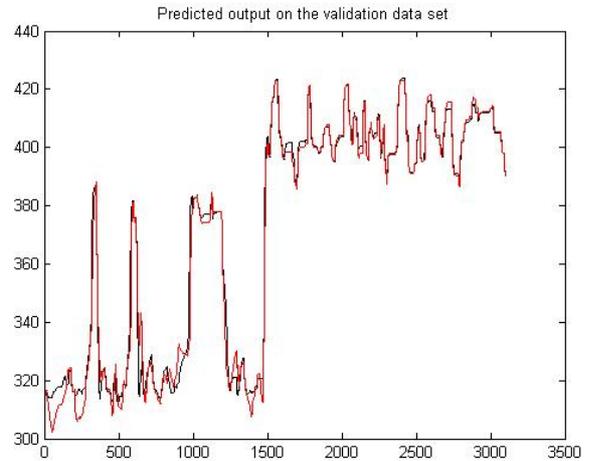


Fig. 4. Temperature Prediction using 8 Linear Models (RMSE = 4.24)

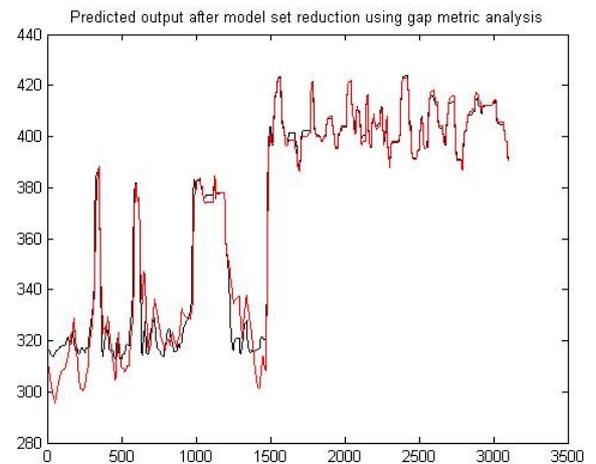


Fig. 5. Temperature Prediction using 7 Linear Models (RMSE=4.64)

After this step, the gap metric analysis is applied on this set of 8 models with  $\delta_{threshold} = 0.1$  and  $PE_{threshold} = 5$ . It was seen that models belonging to clusters 2 and 4 got merged based on the gap metric analysis and total number of models was reduced to 7. The composite prediction using these 7 models is shown in Figure 5. If the closed loop stability criterion is relaxed by setting  $\delta_{threshold} = 0.4$  and  $PE_{threshold} = 9$ , then it is seen that the models belonging to clusters 1,6,7 and 8 get merged into one model; also models belonging to clusters 2,3 and 4 get merged into another composite model. It was also seen that the model belonging to cluster 5 was not similar to any other model in the set. Ultimately, these iterative steps resulted in 3 linear models whose composite prediction is shown in Figure 6. Interestingly, the root mean square error (RMSE) for the cross validation increased from 4.64 to 8.3 when the number of models used in the composite prediction reduced from 7 to 3. Thus it is seen that the choice of the number of partitions need to be judiciously made based on considerations of both prediction error parsimony and stability.

## 5. CONCLUSIONS AND FUTURE WORK

This paper proposes a combination of fuzzy classification based multimodel identification strategy with a gap metric based model set reduction strategy. Together, this combination yields a parsimonious and stable model set which

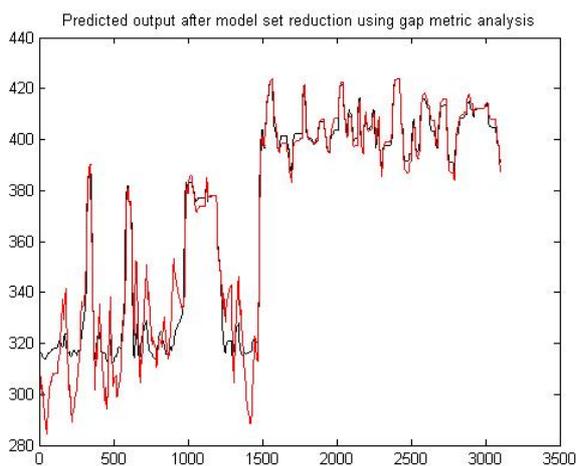


Fig. 6. Temperature Prediction using 3 Linear Models (RMSE = 8.3)

can be used effectively for online control. The application of the proposed methodology on a polystyrene reactor has shown the efficacy of the proposed approach. As the next step the clear guidelines for the specifications of the threshold selection criterion for both the prediction error and gap metric in the model set reduction step, need to be established. The future work should also focus on combining the gap metric based approach with other clustering techniques, as well as extending the approach to include the nonlinear gap metric criterion proposed by (Bian and French, 2005).

#### References

- A., N., Venkat, P., Vijaysai, and R., D., Gudi (2003), Identification of complex nonlinear processes based on fuzzy decomposition of the steady state space, *Journal of Proc. Cont.*, 13, 473-488
- Bian, W. and French, M. (2005), Graph Topologies, Gap Metrics and Robust Stability for Nonlinear Systems. *SIAM Journal of Control and Optimization*, 44 (2). pp. 418-443.
- G., Skarmeta, A., F., Delgado M., and Vila M., A. (1999), About the use of fuzzy clustering techniques for fuzzy model identification, *Fuzzy Sets and Syst.*, 106, 179-188
- Georgiou, T. T., (1988), On the Computation of the Gap Metric. *Syst. Control Lett.*, 11, 253.
- Godfrey, K. (1993), *Perturbation Signals for System Identification*, Prentice Hall International. London
- J., K., Gugaliya, R., D., Gudi and S., Lakshminarayanan (2005), Multi-model decomposition of nonlinear dynamics using a fuzzy-CART approach, *JPC*, 15(4), 417-434
- K., S., Narendra, J. Balakrishnan (1997), Adaptive control using multiple models, *IEE Trans. on Auto. Cont.*, 42(2), 171-187
- P., M., Hidalgo and C., B., Brosilow (1990), Non-linear model predictive control of styrene polymerization at unstable operating points, *Comput. chem. Engng.*, 14(4), 481-494
- O, Galàn, J., A., Romagnoli, A., Palazoglu, Y., Arkun, 2003, Gap Metric Concept and Implications for Multilinear Model-Based Controller Design, *Ind. Eng. Chem. Res.*, 42, 2189-2197

W., K., Wojsznis, T., L., Belvins, M., J., Nixon, and P., Wojsznis (2005), Adaptive multivariable process controller using model switching and attribute interpolation, US Patent No. US20050149209 A1