Supporting Information

Dynamic Nonlinear PLS Modeling Using Gaussian Process Regression

Hongbin Liu[1,3,‡], Chong Yang[1,‡], Bengt Carlsson[2], S. Joe Qin[3], ChangKyoo Yoo[4]*

1. Co-Innovation Center of Efficient Processing and Utilization of Forest Resources, Nanjing Forestry University, Nanjing 210037, China
2. Division of Systems and Control, Department of Information Technology, Uppsala University, Uppsala 75105, Sweden
3. Mork Family Department of Chemical Engineering and Material Science, University of Southern California, Los Angeles, California 90089, United States
4. Department of Environmental Science and Engineering, College of Engineering, Kyung Hee University, Yongin 446701, Korea

Corresponding author: ckyoo@khu.ac.kr

Supporting Information

Dynamic Nonlinear PLS Modeling Using Gaussian Process Regression

Hongbin Liu[1,3,‡], Chong Yang[1,‡], Bengt Carlsson[2], S. Joe Qin[3], ChangKyoo Yoo[4]*

1. Co-Innovation Center of Efficient Processing and Utilization of Forest Resources, Nanjing Forestry University, Nanjing 210037, China
2. Division of Systems and Control, Department of Information Technology, Uppsala University, Uppsala 75105, Sweden
3. Mork Family Department of Chemical Engineering and Material Science, University of Southern California, Los Angeles, California 90089, United States
4. Department of Environmental Science and Engineering, College of Engineering, Kyung Hee University, Yongin 446701, Korea

Table of contents

Combined with the optimal number of latent variables (LVs), Table S1 shows the corresponding tuned parameters for each of the inner relation in D-LSSVM-PLS and D-GPR-PLS models in the BSM1 case.

Table S1. Parameters of D-LSSVM-PLS and D-GPR-PLS models for BSM1 data set

LV	Parameters for D-LSSVM-PLS (Gaussian kernel function)		Parameters for D-GPR-PLS
	Regularization parameter	Kernel width	Parameter p_f
1	9.6	0.5	-132.7
2	3.9	0.2	-404.2
3	47.4	1.1	-244.9
4	0.8	1.8	-407.8

Similar to Table S1, Table S2 provides the tuned parameters for each of the inner relation in D-LSSVM-PLS and D-GPR-PLS models in terms of the BSM1_LT data set.

Table S2. Parameters of D-LSSVM-PLS and D-GPR-PLS models for BSM1_LT data set

LV	Parameters for D-LSSVM-PLS (Gaussian kernel function)		Parameters for D-GPR-PLS
	Regularization parameter	Kernel width	Parameter p_f

1	236.4	0.5	-29.4
2	6.7	0.9	-714.7
3	502.5	1.9	-248.9
4	160.0	2.2	-558.3

Table S3 provides the detailed running times of different models for the prediction of S_{NHeff} and S_{NOeff} in the BSM1_LT case.

Table S3. Comparison of execution time for BSM1_LT data set

Models	Training time (s)	Prediction time (s)
PLS	0.134	0.006
DPLS	0.025	0.005
QPLS	0.110	0.009
D-QPLS	0.131	0.011
LSSVM-PLS	0.267	0.343
D-LSSVM-PLS	0.716	0.449
GPR-PLS	347.498	8.333
D-GPR-PLS	279.640	5.617

Table S4 shows the tuned parameters of D-LSSVM-PLS and D-GPR-PLS models used for effluent chemical oxygen demand (COD) prediction in the WWTP data set.

Table S4. Parameters of D-LSSVM-PLS and D-GPR-PLS models for WWTP data set

LV	Parameters for D-LSSVM-PLS (Gaussian kernel function)		Parameters for D-GPR-PLS
	Regularization parameter	Kernel width	Parameter p_f
1	706.4	11.9	7.8
2	158.3	4.6	-14.6

Table S5 provides the detailed running times of the different models for effluent COD prediction in the WWTP case.

Table S5. Comparison of execution time for WWTP data set

Models	Training time (s)	Prediction time (s)
PLS	0.015	0.004
DPLS	0.017	0.004
QPLS	0.066	0.005
D-QPLS	0.062	0.006
LSSVM-PLS	0.012	0.010
D-LSSVM-PLS	0.014	0.010
GPR-PLS	2.039	0.021
D-GPR-PLS	1.931	0.023

Figure S1 illustrates the variations of the industrial wastewater treatment process (WWTP) after data pretreatment.

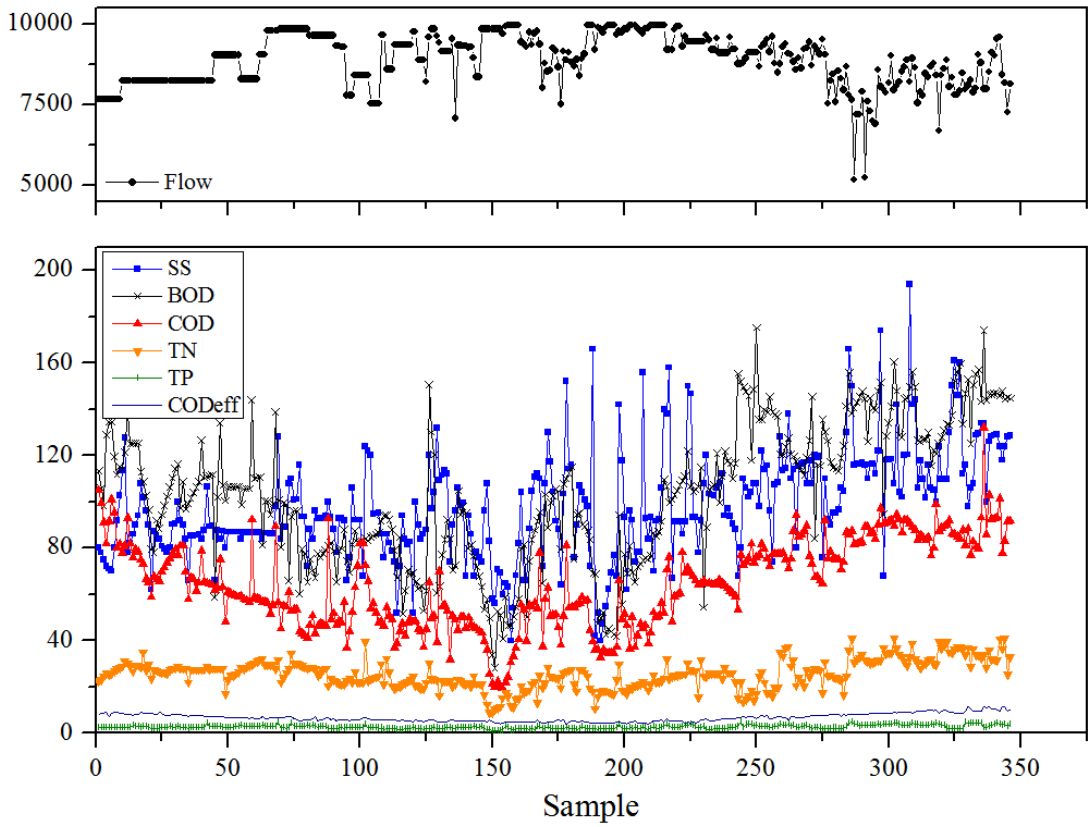

Figure S1. Variations in the industrial WWTP data set