Partial Least Squares Random Forest Ensemble Regression as a Soft Sensor

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Abstract

Six simple, dynamic soft sensor methodologies with two update conditions were compared on two experimentally-obtained datasets and one simulated dataset. The soft sensors investigated were: moving window partial least squares regression (and a recursive variant), moving window random forest regression, feedforward neural networks, mean moving window, and a novel random forest partial least squares regression ensemble (RF-PLS). We found that, on two of the datasets studied, very small window sizes (4 samples) led to the lowest prediction errors. The RF-PLS method offered the lowest one-step-ahead prediction errors compared to those of the other methods, and demonstrated greater stability at larger time lags than moving window PLS alone. We found that this method most adequately modeled the datasets that did not feature purely monotonic increases in property values. In general, we observed that linear models deteriorated most rapidly at more delayed model update conditions while nonlinear methods tended to provide predictions that approached those from a simple mean moving window. Other data dependent findings are presented and discussed.

Keywords: Soft-Sensor, Random Forest Regression, PLS regression, Model fusion

1. Introduction

Soft sensors for regression tasks have found wide utility in process engineering. A soft sensor is effectively a calibration used on time-series data.

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Here, we consider a soft sensor to be any algorithm that can be used to infer a property value from several measurements. The goal of implementing a soft sensor is to avoid implementing a physical sensor for quality variables that may require extensive time or work up to measure[1]. In the context of industrial chemical processes, these algorithms should meet several specifications. In most situations, soft sensors need to be able to process multivariate data quickly and should also be able to predict a property of interest despite delayed or infrequent laboratory reference measurements [1].

There are several general approaches to soft sensing that satisfy these requirements. One of the most common approaches is the use of local regression models of the process. Local models are a collection of several calibration models that are applicable to data collected at a specific region in time, such that each calibration corresponds to only a portion of the physical process or mode. Due to the complexity of chemical process data, model efficacy often deteriorates when any change occurs in a process. Thus, local models are typically tethered to a classification-like step, so that the process mode can be identified and an appropriate calibration can then be applied to only a specific set of process samples. Several notable examples of mode identification include ones based on finite mixtures of Gaussian models [2] and mixtures of partial least squares ensembles [3]. These local modeling methods have been shown to work well, but often feature complicated implementations, leading to relatively large models.

The use of large local models can be seen as restrictive for a real world chemical process. For example, consider a process where 1000 reference measurements are required to build each local calibration model, where the process duration is a total of 10,000 time points, and where the reference value requires a 10+ minute gas chromatographic analysis. In this example, a soft sensor would require seven or more days to develop a model for any new process mode. The cost of identifying a local mode incorrectly could, in some cases, become detrimental to process safety or efficacy due to the large proportion of down time. Despite that, locally-modeled soft sensors may be effective for a given chemical process, but there is no guarantee that they are applicable to future iterations of the same process.

A different approach, which bypasses issues of online mode identification and adaptive modeling, is to build the process model from off-line historical data and apply it to online data[4 5]. This method has been shown to work for simulated data sets. However, real processes can feature unpredictable phenomena or subtle process changes (sensor drift, sensor replacement, etc),
that may not have been encountered in the historical data and are therefore not part of the model. These unanticipated effects in the process can render a soft sensing model inaccurate [6]. However, using a model based on historical data does avoid difficulties with the sensor being down during training, because this model is trained off-line.

In this work, we present and compare the predictive accuracy of several soft sensing strategies for regression tasks based on local models without relying on either process mode identification or on historical data. The models presented in this study are developed under the assumption that laboratory reference measurements can be updated throughout the process but only require a few sample measurements to begin predicting on new data. These models are also easy to implement with modern software packages. We introduce, for the first time, a soft-sensor ensemble based on the combination of random forest regression (RF) and partial least squares regression (PLS), which can be used in real-time applications for one- or several time-step ahead predictions used in process modeling.

2. Theory

2.1. Soft sensing

Soft sensing is a form of multivariate calibration used to relate property values to indirect measurements made on a multivariate time series. Soft sensors are typically models based on physical measurements (temperature, pressure, etc) of a process to infer chemical properties (concentration, purity, activity, etc). Because of the similarities between soft-sensing and multivariate calibration, standard modeling techniques, such as partial least squares regression (PLS) can be used for soft sensing, with some adjustments.

2.2. PLS

Partial least squares regression is a regression technique commonly employed in chemometrics [7]. Like traditional least squares regression, dependent observations \( y \) are regressed onto independent measures \( X \) using the standard linear form, \( y = X\hat{b} + \epsilon_y \), where \( \hat{b} \) represents the regression coefficients, and \( \epsilon_y \) is the residual error from the fit to the corresponding true \( y \) vector. However, in PLS, unlike multiple linear regression, the regression coefficients are constructed from a bilinear decomposition of the covariance
between $y$ and $X$,  
\begin{align*}
y &= uQ^T + e_Y \\
X &= TP^T + E_X
\end{align*}

(1)

where $u$ and $T$ are the projections (scores) from $y$ and $X$ onto the mutually orthogonal axis loadings $Q$ and $P$, respectively. By convention, most models are constructed to predict $y$ from measurements contained in $X$. However, both equations are required because the loading axes for $Q$ and $T$ are obtained from decompositions of the $X^Tyy^TX$ matrix, such that the covariance between $T$ and $u$ is maximal. The estimated regression coefficients $\hat{\beta}$ are calculated from both equations via the weights ($w$) of the projection from $T$ to $P$, $\hat{\beta} = wQ^T$.

The orthogonal nature of the PLS scores removes collinearity from the $X$ data and allows for dimension reduction. These two features are a notable advantage over many other regression methods and because of this, PLS has been shown to be well-suited for many regression tasks. However, for time-dependent data, the covariance of $X$ often changes with time in unpredictable ways. Therefore, the usual static calibration models developed from PLS are not suited to soft-sensing.

2.3. Moving Window PLS

One simple adaptation to make any static, multivariate calibration method more responsive to changes in the autocovariance of the time-dependent data in $X$, is to employ a moving window. Many variations on this approach have been reported [8, 9], but only the simplest case that of modeling a time-series with a moving window is examined here. A window, a collection of adjacent samples with known property values, is selected for calibration. The local calibration model built on a window of time-dependent data can be used to predict properties of samples collected at future time steps.

To account for changes in the covariance of time-dependent data, the window can then be moved one or more time steps ahead and a new calibration model can be trained on those samples now in the calibration window, provided reference measurements exist. This sequence of modeling and prediction can be repeated for any number of incoming samples. We refer to the case where the modeling window is moved forward by one time step after every prediction as the "continuously updated case". In a similar way, we refer to the "delayed update case" as the case where the calibration model,
or window, is updated less frequently than every time step. These two cases are shown in Figure 1.

Figure 1: Cartoon depictions of models which are continuously updated (above) and those which are updated with a delay (lower). The horizontal axis depicts samples and their temporal order, and unlabeled boxes indicate the samples used to construct models, while boxes that are labeled with "?"s are the samples of property values for prediction. In the continuous case the sampling window moves with a fixed number of samples prior to the sample for prediction; in this example the window is one time step behind the prediction sample. While in the delayed update case, several samples are predicted from one window location before the window is updated and moved. In this example the window size is three time steps, and the window predicts upon two samples before it is updated.

Although the moving window approach can be used to overcome time-related changes in the autocovariance, this approach does not permit the regression model developed for the window of data to retain information from samples collected prior to the window. Please note, this moving window modeling approach to handle time dependent data differs from the variable selection technique called moving window PLS, often abbreviated as MWPLS[10].

2.4. Recursive PLS

One adaptation to PLS that allows modeling of time-series data is to make its model inputs recursive. Recursive model adaptation allows information from previous times to be used in the current sample window. This idea was first pioneered by Helland et. al to make the PLS framework more amenable to time-dependent data [11].

Qin et. al. [8] showed that PLS algorithms which normalize the X score vectors (T), but not the weights or X loadings (P), can be made recursive.
The recursive algorithm modifies the \( X \) and \( y \) input matrices to incorporate information from the previous PLS model and newly obtained data (\( X_{\text{new}}, y_{\text{new}} \)),

\[
X = \begin{bmatrix} \lambda P^T_{\text{old}} \\ X_{\text{new}} \end{bmatrix}, \quad y = \begin{bmatrix} \lambda B_{\text{old}}Q^T_{\text{old}} \\ y_{\text{new}} \end{bmatrix}
\]  

(2)

where \( B_{\text{old}} \) represents a diagonal matrix of inner model coefficients which are defined as, \( u \times T \), and where \( \lambda \) is a scalar forgetting factor. The forgetting factor determines the relative amount of information retained from previous models in the recursive update. Qin’s method allows for new information to be incorporated into a weighted PLS model in an adaptive manner.

2.5. Artificial Neural Networks

Although both moving window and recursive PLS models can be used to handle changes in the autocovariance of the multivariate \( X \) data, in both cases the underlying regression models are linear. It has been suggested that the relationships between regressors and predictors measured over long periods of time are nonlinear and might be better modeled by an artificial neural network. Artificial neural networks have been widely used to learn nonlinear relationships from complicated patterns in very large feature and/or sample spaces. The literature which pertains to neural networks, and neural networks for soft sensing, is vast. This is largely a result of the mathematical proof which shows that a single-layer neural network can learn any arbitrarily complex relationship\[12\]. We only briefly survey the single-hidden-layer, feedforward neural network (FFNN) topology as it pertains to two of the models used in this study. For a review of neural networks as they have been applied in the field of chemometrics, see Marini, et al. \[13\]

A feedforward neural network was selected for this study because of its wide use in soft-sensing and its simplicity when compared with that of the many high-level neural network architectures. Feedforward neural networks are composed of many processing units, or neurons, and sometimes several layers of those neurons. A layer, in the context of feedforward neural networks, is a collection of neurons and the mathematical operations which are subsequently performed. Each fully connected neuron maps the output from the previous layer (starting from the input layer or \( X \)) by the dot product with the learned weights (\( W \)) and the sum of their learned biases (\( \theta \)) into the next layer (\( Z \)). This constructs a linear mapping where the output of the entire hidden layer has the form \( Z = WX + \theta \). A nonlinear transfer, or
activation, function is usually applied to $Z$ to incorporate nonlinearity and bound the neuron weights between zero and unity for model stability. In this study a sigmoid activation function was applied to the output of each hidden layer neuron ($A(Z) = \frac{1}{1+e^{-Z}}$) and the output layer (or prediction), used a linear activation function.

The output from the activated hidden layers were fed into a linearly-activated ($A(Z) = Z$) fully-connected single neuron layer which output a scalar predictor value. The use of linearly-activated output layers is common in neural networks used for regression tasks because the output is not bounded and provides a prediction over a continuum of possible values.

The weights and biases in the hidden layers of a neural network have usually been computed by a process called back-propagation. Back-propagation is used to estimate how the error in a prediction propagates backwards through the network layers with respect to each neuron and its activation function. The task is accomplished by adding small perturbations to the weights in the direction which minimizes the error or the loss function via backward mode differentiation. The back propagation process is repeated until a set number of iterations, or epochs, have been completed. The loss function employed in this study was the mean squared error, $MSE = \frac{1}{N_{\text{observations}}} \sum (y_{\text{predicted}} - y_{\text{actual}})^2$, as it is most suitable for regression tasks and is more cheaply computed than the root mean squared error ($RMS\!E = \sqrt{MSE}$). In this study a simple, stochastic gradient descent optimizer with a fixed learning rate of 0.005, and no other hyperparameters, was employed to find optimal weights and biases for every layer in the neural network models used.

One notable advantage to NN models for soft sensing is that neural networks can be updated easily. Rather than rebuilding a model with new data, as in the case of a moving window-based regression, any trained feedforward neural network model can be back propagated with new data and retain information from previous time points in the weights and bias terms. For the aforementioned reasons neural network approaches have been popular in soft sensor research. We found in updating the models as new sample measurements became available, that back-propagating for 75 epochs was sufficient for predicting on future data.

2.6. Random Forest Regression

Although updating a neural network can be easily performed, other non-linear regression techniques can also be employed. One of the simplest is that
of a regression tree. Breiman’s classification and regression tree algorithm (CART) [15] has received a lot of use for classification, but its suitability for nonlinear regression is less often mentioned. CART trees are widely used in classification tasks for their simple interpretations and ability to model nonlinearities in data. For regression, however, CART trees possesses several weaknesses. To describe the strengths and weaknesses of the CART algorithm and later motivate the use of random forest models, a brief review of regression trees is provided below.

Regression trees are collections of sequential binary decisions, where each decision pertains to a selected independent variable. For example, assume that the matrix \(X_{o,c}\) contains \(o\) row-wise observations and \(c\) columns or variables. A regression tree model operates by selecting a variable \(v\) from \([1, c]\), and two observations, \(r_1\) and \(r_2\), in \(o\) to create a decision boundary from the mean of \(r_1\) and \(r_2\). The decision boundaries are then used to partition the remaining samples into two groups, depending on whether each sample is greater or less than \(\frac{r_1+r_2}{2}\).

The variables and observations for each partition which create the decision boundary are selected such that a gain metric is maximized. The gain metric commonly used for regression trees is the sum of squared errors for prediction, defined as \(SSE = \sum (y_{predicted} - y_{actual})^2\). This gain metric is unlike the gain metrics used in classification trees. Classification trees use a metric such as GINI, which measures gain as a function of class purity at each node and branch[15]. The process of sample partitioning is then repeated in a recursive manner on each partition until a stopping condition is met. The most common stopping criteria for regression trees is reached when either the act of introducing a new decision or partition no longer organizes the samples into distinct groups which have similar property values or when the number of samples in a given partition is less than a user-specified percentage.

Predicting from regression trees is easily accomplished after the tree has been constructed. New samples are passed through the hierarchy of binary decisions until the samples are described by the set binary decisions created from the training samples. At this point, the samples are assumed to possess the same property value as the samples that populate terminal node, or "leaf", of the regression tree. Predicting from decision trees is computationally efficient relative to many other methods because all that is required is that variables and decisions are stored along with the property values at each terminal node.

Although regression trees are fast to train, there are problems with the use
of a single regression tree for a complex regression task. Decision boundaries constructed from minimizing the squared errors of prediction will tend to grow overly complex trees. Every unique instance of a property value will tend to result in its own terminal node. Thus, the decisions made on future data will be over-fit to the training data and will often appear discrete, in contrast to the notion that regressions should be able to interpolate between property values on which the model was trained with. In the form presented above, a regression tree can only predict values used in training.

There are many schemes to overcome this issue, each with their own strengths and weaknesses. Some notable examples include implementing piecewise least squares regression at tree nodes [14], and pruning [15]. The approach taken here was to grow many trees, each being made from a random selection of variables and training samples contained in a moving window. The average of the predictions from many trees with stochastically-selected variables and samples tends to be a reliable estimate of the property value [16]. This process of randomly sampling variables and observations is called bootstrap aggregating or bagging [17].

The technique of combining predictions from many regression trees via the use of bagging is referred to as random forest regression. We utilized random forest regression on a moving window, as presented in the PLS case, for soft sensing. Much like CART, Breiman’s Random Forest algorithm is widely known for classification, but its utility for nonlinear regression is less often mentioned. Random forest regression is not commonly used for soft sensing, but a recent article reported that the performance of a random forest ensemble model was similar to that of a neural network for determining waste water quality from processing plant sensors [19].

2.7. Random Forest Partial Least Squares Regression Ensemble Modeling

Although the random forest technique is widely used in classification for its ability to robustly handle noise and to model nonlinearities in data [18], random forest modeling possesses a notable weakness for regression. Even though random forest modeling can be used to interpolate between training sample property values on new data: it cannot be used to predict property values beyond those in the range that it was trained upon.

To extrapolate predictions outside of the values contained in a training set, as in PLS, while also incorporating an ability to handle nonlinearities in changes across the covariance, such as in RF, a novel combination of both methods was created. Random forest partial least squares ensemble models
are made by incorporating PLS prediction(s) of the unknown sample as well as the measured reference samples which are typically included in a moving window model into a single random forest regression model. This is shown diagrammatically in Figure 2. The introduction of PLS samples allows for the linear prediction from one or more PLS models to, potentially, extend the range of prediction in a random forest.

Figure 2: A depiction of how the random forest partial least squares regression ensemble is constructed. PLS models are created from samples collected prior to the unknown and their predictions are used along with known samples information to construct a random forest regression model. This model is then used on unknown data to predict its property value.

Predicting from the random forest partial least squares ensemble model is then performed by inputting the X information from the unknown sample into the random forest model. Updating the ensemble model to predict upon new samples is analogous to that of the moving window. Both the PLS and random forest sample windows are reconstructed from samples which are one or more time steps forward to create both the PLS and RF models.

Information leakage arising from training on test data, does not occur with a proper implementation of this algorithm. Although the random forest
regression models are constructed from PLS predictions onto the unknown sample, the PLS inner models do not contain the actual $y$ value, only one or more moving window PLS predictions of it. Similarly, the raw $X$ data which is also incorporated always precedes the unknown sample.

3. Data

3.1. Debutanizer process

The debutanizer process data were collected from a distillation column which was designed to remove butane from gasoline. The goal of the process was to quantify the amount of butane in gasoline as it was refined. Butane amounts (2394) were inferred from measurements (7) of temperature at the top of the column ($v_1$), at the bottom of the column ($v_6, v_7$), in the sixth tray ($v_5$), the redux flow ($v_3$), the flow to next process ($v_4$), and pressure at the top of the column ($v_2$) [20].

The property values for this dataset were lagged by 8 samples to account for the time mismatch between soft sensing and butane quantitation. The sensor data were collected at a fixed time interval, of 6 minutes, but the reference measurements took considerably longer to collect, 45 minutes. For model predictions from the sensor data to relate to property values at an appropriate time and to avoid building models which predicted butane concentrations collected 39 minutes prior to the current measurement, the property values were lagged by 48 minutes so that predictions from nearly real-time sensor information could be made.

3.2. Sulfur Recovery Unit Process

The Sulfur Recovery Unit (SRU) process was designed to neutralize $\text{H}_2\text{S}$ and $\text{SO}_2$ gasses and to retain elemental sulfur from furnaces in a chemical plant. The process utilized 5 gas flow sensors which collected measurements every minute so that the concentrations of both sulfurous gasses could be inferred [20]. The SRU data has many instances where consecutive property values have exactly the same numerical value. An artificial floating point precision offset ($1\times10^{-6}$) was added to every $y$ value that was identical to its earlier neighbor to avoid zero-variance data, which would otherwise cause partial least squares regression modeling to fail when applied to data in short process windows.
3.3. Simulated Penicillin Fermentation

We also examined data from a simulated penicillin fermentation process. The process data consisted of 15 variables: aeration rate, agitator power, substrate feed rate, substrate feed temperature, acid flow rate, base flow rate, cooling water flow rate, substrate concentration, dissolved oxygen concentration, biomass concentration, penicillin concentration, culture volume, carbon dioxide concentration, pH, fermentor temperature, and generated heat [21]. The goal was to infer the penicillin concentrations from the other process variables. With the exception of the sampling interval (1.1 hrs) and simulation time (350hrs), all of the settings that were utilized in the simulation were the default settings. This dataset served as a negative experimental control because, unlike the debutanizer and SRU data, the property value had a monotonically increasing trend.

4. Methods

Partial least squares regression and random forest regression were the moving-window-based methods selected for this study. The mean of the moving window was implemented as a negative experimental control. The mean moving window model assumes that an unknown property value is the average property value of the window of \( w \) samples which proceeded it, \( y_t = (y_{t-1} + y_{t-1} + ... + y_{t-w}) \). The mean prediction of a moving window was implemented as a control because an estimate from the mean moving window assumes that all future predictions are expected to resemble their neighboring samples, and makes no use of the underlying structure in \( X \). An effective soft sensor model should always outperform any model that does not incorporate information presented in \( X \), in time-dependent changes in \( y \), or in how \( y \) changes with respect to changes in \( X \).

Feedforward neural networks and recursive PLS regression were selected as adaptive methods to be compared with the moving window techniques, so that results from two commonly used techniques could be compared with those from the novel random forest partial least squares ensemble. The feedforward neural network model topologies were tuned to achieve low predictive errors. For the debutanizer process data, as suggested by the original reference [20], we employed an autoregressive feedforward neural network. The network model incorporated previous \( y \) data into the \( X \) matrix via, \( y(t) = f(v_1(t), v_2(t), v_3(t), v_4(t), v_5(t), v_5(t-1), v_5(t-2), v_5(t-3), v_6(t) + \)
\[ \frac{v(t)}{2}, v(t - 4), v(t - 5), v(t - 6) \] [20], where \( v \) and \( t \) represent the independent variables and time, respectively. The feedforward neural network topologies for each of the datasets used are provided in Table 1.

Table 1: The number of neurons per hidden layer for each feedforward neural network used in this study. Layers denoted with '-', did not contain nodes in the specified hidden layer.

| Data set     | Number of Neurons | Number of Neurons | Number of Neurons |
|--------------|-------------------|-------------------|-------------------|
|              | Layer 1           | Layer 2           | Layer 3           |
| Debutanizer  | 4                 | 8                 | 16                |
| SRU H₂S      | 50                | -                 | -                 |
| SRU SO₂      | 50                | -                 | -                 |
| Penicillin   | 35                | 70                | -                 |

Both of the previously mentioned updating approaches, the continuously updated case, and the delayed update case with varying update frequencies, were investigated for each technique and each dataset. The window sizes used for the models were determined empirically, as described below.

5. Results and Discussion

An experiment to determine the relationships, if any, between the predictive error and moving window size was performed on all of the datasets. The mean moving window predictor, PLS, RPLS, and RF models were used with window sizes of 2-10, 15, 20, and 25 samples (Figure 3) in order to assess the predictions of the property value for the sample that immediately followed the window for every sample. It was observed that across a given dataset as the window size increased, so did the prediction error.

The relationship between window size and errors of prediction was anticipated but stands at odds with that seen from typical multivariate calibrations done on static data. The effect of using small sample sizes to build traditional multivariate calibration models is well known. Typically, small training sets fail to span all sources of variance and introduce biases; these lead to calibration models that are not robust to noise or background effects. Because of the latter, a challenge problem with very few samples was introduced in 2007 for a chemometrics conference [22]. However, the prediction errors reported in this study are local models, in that, they are only predicting one-sample-ahead of their window. In three of the datasets local changes
The finding that small window sizes performed better than large ones on the other 3 datasets was the basis for the development of models used throughout the rest of the study. We selected a window size of 4 for the PLS, RF, and RPLS methods used in the remaining studies because it tended to perform well. This window size also did not tend to reduce the local PLS models to least squares regression by having the optimal number of latent variables be the same as the rank of the sensor data contained in the cross-validated sample window. The PLS-RF models performed best by utilizing information from only 2 samples prior to the unknown sample and a PLS prediction made from the previous 3 samples onto the unknown.

The root-mean-square errors of prediction for one-time-step-ahead predictions were examined (Table 2). For the debutanizer data, we found that an RF-PLS model had a predictive error (1.44%) which was competitive with a recently reported and more complex least-squares support-vector-machine based (LS-SVM) soft sensor (1.20%) [23]. Similarly, we found that our new method, and several of the comparison methods had lower errors of prediction than a LS-SVM(H_2S = 3.97%, SO_2 = 5.12%) and relevance vector
machine (H$_2$S = 4.01%, SO$_2$ = 5.11%) model on the SRU data. However, the errors from the literature sulfur recovery unit data example and ours are not directly comparable, because the authors made a static model from 1680 samples before regressing on a selected set of 1680 samples out of the total 10,080 samples available. The work reported here considered all of the data. It was also observed that the RF-PLS method reported here had a lower RMSEP than that of the moving window RF on all of the datasets studied, a result which indicated that the incorporation of PLS predictions into the RF model was beneficial. The RF-PLS method also featured the lowest prediction error for the property values of the debutanizer and SRU data.

Table 2: Root mean squared errors of prediction of all the methods studied on the debutanizer and sulfur recovery unit datasets for one-step-ahead predictions. Entries in bold indicate the lowest RMSEP for a given dataset, and those in italics were the second lowest.

|                      | Debutanizer (RMSEP %) | SRU H$_2$S (RMSEP %) | SRU SO$_2$ (RMSEP %) |
|----------------------|-----------------------|----------------------|-----------------------|
| RF                   | 2.43                  | 2.60                 | 2.79                  |
| PLS                  | 1.58                  | 2.16                 | 2.30                  |
| RPLS                 | 2.90                  | 2.39                 | 2.62                  |
| RF-PLS               | **1.44**              | **1.91**             | **2.06**              |
| FFNN                 | 2.61                  | 3.03                 | 3.09                  |
| Mean-Moving-Window   | 3.14                  | 3.06                 | 3.26                  |

A comparison of the methods with the experimental control, the mean-moving-window method, provides some insight on the performance of the methods for one-step-ahead predictions. No instances were observed where any of the 5 models had a greater RMSEP than the mean-moving-window for one-step-ahead predictions, suggesting that all of the methods used information in the X matrix to model y better than the mean-moving-window model. This result was anticipated, even though the debutanizer data features large regions of monotonic trends in the property value. While random forest regression cannot be used to predict property values outside of its training sample range, random forest regression can impart an upwards or downward bias in its predictions relative to the mean value of previous samples, which may not accurately model a process, but still more closely resembles the actual value. The FFNN also outperformed the mean-moving-window predictions, but this method had larger one-step-ahead predictive
errors than those from random forest regression in every test instance. Although there are many reports where nonlinear models are applied to time series data without the incorporation of linear elements, these models tended to perform poorly with small window sizes for one-step-ahead predictions on the datasets studied here.

While there is merit in being able to predict one-time-step ahead, and to do so with low error, we focused on predicting several time steps ahead. In almost any experimental setting, there is a possibility of human or process error occurring. Many cases where a sample analysis could be delayed by one or more sampling times could be envisioned. Two cases for handling such events were investigated. The first case, a delayed update, is when the process model is not updated until the next window size of samples becomes available. The second case, a continuous update, is when updates to the model are performed as soon as the next measured value becomes available. The one-time-step ahead predictions can be seen as the degenerate solution to updating for either a model that is updated at every single time-step, or predicting ahead from a window by 1 time-step delay. Both update conditions were investigated for the remaining three data sets at different time delays for model update.

Figure 5 shows the errors of prediction that were obtained from the debutanizer and sulfur recovery unit data sets under the delayed update conditions. Within the range of one to nine time-step lags for model updates, the following modeling methods were observed to provide predictions worse than those obtained from the mean value modeling on more than one dataset: PLS, RPLS, and FFNN. Both the RF and RF-PLS modeling methods were more robust to time lags before window updates. RF-PLS and RF models were not observed to perform worse than the mean predictor. This finding gave evidence to suggest that the random forest based inference on these datasets was always better suited to prediction than a model which did not incorporate information from $X$.

Relative to the random forest regression method performance gains were achieved by including PLS predictions into the RF models (RF-PLS). In all but one (out of 27) update conditions on all datasets, predictions from RF-PLS were better than those from RF alone. RF-PLS models produced lower RMSEP values than those from PLS. This result indicated that predictions from PLS were improved by incorporating a moving window of samples inside of the random forest algorithm. Overall RF-PLS tended to present the lowest errors of prediction for these datasets under the delayed update condition.
The continuously updated case assumes that a window of process measurement samples is always delayed one or more time steps behind a sample for prediction. The continuously updated models tended to have greater predictive errors than those found using the same models when the delayed update case conditions were imposed as can be seen in Figure 6. This result was expected because the continuously updated models have a longer time delay from the currently available sample window to prediction than that of the delayed case. For example, if both update conditions are set to have an update of 4 sample-steps, the continuous delay window is always predicting 4 samples ahead of its window for each of the 4 samples, while the delayed update predicts 1, 2, 3 and 4 samples ahead of its window for the same samples. On average, at time delays greater than one time step, the delayed update has more training samples closer to the samples it predicts upon, and can form better predictions. The increase in performance is because the training samples information are local relative to the unknown sample. For the continuously updated condition, only the random forest regression method produced better predictions than the mean-moving-window model in all datasets and over all time lags investigated.

For the debutanizer data, the RF-PLS ensemble model afforded the lowest error of prediction for all nine time lags. However, when applied to the SRU data, random forest partial least squares regression only offered the lowest
error of prediction until the 4th time lag. When lagging the model window 4 time steps from its prediction, only RF modeling afforded predictions better than those obtained from the mean-moving-window model. The most notable benefits from combining the PLS and RF predictions in the SRU dataset occurred at lower time lags. However, the increase in error of prediction for larger time lags (5-9) from RF-PLS modeling was much lower on the SRU data than that of PLS or RPLS modeling. The errors in prediction most closely resembled RF modeling. The fact that errors from random forest partial least squares regression approached those obtained from the mean-moving-window predictor for time lags in situations where it failed to afford the lowest error is a promising trait for a soft sensor.

Overall, the random forest regression models appeared to perform better than the mean-moving-window model. Although it performed well at large time lags, the mean-moving-window model performed poorly at shorter time lags relative to the other modeling methods. In an industrial process where a moving window is applicable, and where the goal is to predict only a few samples ahead of the measurement of a property, partial least squares regression appears to be a good choice. However, after combining PLS and RF modeling, lower one-step-ahead predictions, and on one dataset, lower overall predictions were observed than those from partial least squares regression. Perhaps most importantly, when the RF-PLS model failed to produce the
best results, it was never more than 3% different than the mean-moving-window prediction. In the majority of instances, regardless of the updating conditions (97.77% of trials), the combination of PLS and RF in the RF-PLS ensemble provided a lower predictive error than either PLS or RF alone.

Although the random forest partial least squares ensemble model technique showed promise on all of the property values available in the debutanizer and the sulfur recovery unit data, it performed less well on the penicillin data set. The penicillin process data had one notable feature that distinguished it from the other datasets. Unlike the other property values studied here, the concentration of penicillin was observed to monotonically increase as can be seen in the supplementary information. The penicillin process was used as a means to assess how well RF-PLS could model a monotonically increasing property value; it was expected that random forest regression models would perform poorly under monotonic changes.

The inversely proportional trend between window size and modeling accuracy that was observed on the debutanizer and SRU datasets was not seen with partial least squares regression and recursive PLS on the simulated penicillin dataset (Figure 6). On the penicillin data the PLS-based models, at least within the range of window sizes examined, a larger window size led to lower errors in prediction, probably because of small or infrequent changes in the $X$ covariance structure. The nearly uniform error produced by RF modeling on this process data can be explained by the fact that random forest regression cannot be used to predict values beyond the training range. The predictions made from the random forest regression moving window models were always lower than the value to be predicted because the property values were monotonically increasing. The penicillin dataset was considered an outlying dataset for the RF-PLS model because there was little benefit to incorporating a random forest model on this dataset.

Both updating conditions, the continuous and delayed updates, were examined first on the penicillin fermentation, or outlying, dataset (Figure 4). The PLS modeling methods provided the lowest error for both model update cases at all delay frequencies studied. Again, the random forest modeling method was unable to predict values outside of those from the process data contained in its training window, and had systematic negatively biased predictions as a consequence. Although the coupling of PLS prediction with the prediction window for the RF-PLS method did produce uniformly lower errors of prediction than those obtained through the use of RF alone, RF-PLS modeling did not perform as well as either of the other PLS methods. For
datasets similar to the penicillin fermentation data one could expect that PLS methods would be better suited. The nonlinear modeling technique, the FFNN model, was the only model which resulted in prediction errors that were greater than those from the mean moving window control for this dataset.

We believe that the feedforward neural network models were hindered by the range of the training data in a way that is similar to random forest regression. The first hidden layer of these networks consists of a dot product much like that of linear regression, and could be used to predict outside of the training set. However, the nonlinear activation functions constrain the dot product between $X$ and the weights to be between zero and unity before the information is transferred on to a subsequent layer. For this model, the sigmoid activation function likely restricts weights from extrapolating results which are much greater or lesser than the samples in a training set. A commonly used remedy for this is to use rectified linear unit (ReLu) activation functions ($A(Z) = \text{max}(0, Z)$), so that there are no upper bound restrictions
imposed on the weights, but experiments performed with ReLu activations afforded less stable results, with greater errors of prediction, than the models that are presented here which used sigmoid activation functions.

The penicillin data illustrated a data set where modeling with feedforward neural networks, random forest, and the random forest partial least squares ensemble did not produce low errors of prediction. Different trends were observed with relation to the modeling error and time lag before updates were observed for the other data sets, none of which had monotonic $y$ structures. The penicillin data was included in this report to demonstrate a worst case where the RF-PLS modeling technique could be expected to perform poorly. Interestingly, predictions from RF-PLS modeling still out performed random forest regression and the feedforward neural networks in both window update conditions, and with respect to its one-step ahead errors of predictions (Table 3).

| RMSEP (g/L) | 0.0102 | 0.0035 | **0.0014** | 0.0081 | 0.0108 | 0.0131 |
|-------------|--------|--------|------------|--------|--------|--------|

### 6. Conclusion

Considering all of the results from these experiments we found that although the nature of the data was an important factor in the success of the models studied, so were the model update conditions and window sizes used. We found that, by using small window sizes, PLS, RPLS, and RF regression models offered low predictive errors relative to those obtained by using larger window sizes in the modeling. On comparison with several literature examples with cutting edge soft-sensor methods, the one-step-ahead errors we obtained with these simple methods were, on both property values of the sulfur recovery unit data set, lower and in the worst case could be seen as competitive. Interestingly, the adaptive mechanisms either recursively updated models (RPLS) or models retrained on new instances (FFNN) tended to produce poorer predictions than recreating an entire model on a small window of samples for two of the datasets. The new soft-sensing method, RF-PLS,
was the most robust to time lag between its window and its unknown sample while still featuring the lowest error for one step ahead predictions on three of the datasets reported here. Its application to modeling processes which have monotonic property values appeared limited, much like random forest regression. On processes that were not entirely monotonic, such as the debutanizer or sulfur recovery unit data, the RF-PLS models offered the lowest predictive errors in the delayed update case, and in most instances, in the continuously updated case. On datasets that did not have monotonic trends in $y$, the combination of random forest regression and partial least squares was in the majority of update conditions more beneficial than either separately.

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8. References

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9. Supplemental Information

Figure 7: Relative amount of butane through out the debutanizer process.

Figure 8: Relative amounts of SO$_2$ through out the sulfur recovery unit process.
Figure 9: Relative amounts of \( \text{H}_2\text{S} \) (below) throughout the sulfur recovery unit process.

Figure 10: Simulated concentration of penicillin throughout the penicillin fermentation process.