Sparse Incremental Regression Modeling Using Correlation Criterion with Boosting Search

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Abstract—A novel technique is presented to construct sparse generalized Gaussian kernel regression models. The proposed method appends regressors in an incremental modeling by tuning the mean vector and diagonal covariance matrix of individual Gaussian regressor to best fit the training data based on a correlation criterion. It is shown that this is identical to incrementally minimize the modeling mean square error. The optimization at each regression stage is carried out with a simple boosting search. Experimental results obtained using this technique demonstrate that it offers a viable alternative to the existing state-of-art kernel modeling methods for constructing parsimonious models.

Keywords—Regression, Gaussian kernel model, incremental modeling, correlation, boosting

I. INTRODUCTION

A basic principle in nonlinear data modeling is the parsimonious principle of ensuring the smallest possible model that explains the training data. The state-of-art sparse kernel modeling techniques [1]–[10] have widely been adopted in data modeling applications. These existing sparse modeling techniques typically use a fixed common variance for all the regressors and select the kernel centers from the training input data. We present a flexible construction method for generalized Gaussian kernel models by appending regressor one by one in an incremental modeling. The correlation between a Gaussian regressor and the training data is used as the criterion to optimize the mean vector and diagonal covariance matrix of the regressor. This approach is equivalent to incrementally minimizing the modeling mean square error. The optimization is carried out with a simple boosting search. Because kernel means are not restricted to the training input data and each regressor has an individually tuned diagonal covariance matrix, our method can produce very sparse models that generalize well and it offers a viable alternative to the existing state-of-art sparse kernel modeling methods.

Our proposed incremental modeling method is very different from the cascade-correlation incremental learning [11]. In the cascade-correlation method, regression units are constructed on a variable space of increasing dimension, namely, the inputs to a unit being the original inputs and the outputs of the previously selected units. Our proposed method is a truly incremental modeling from the input space to the output space. It has a desired geometric property that a regressor is constructed to fit the peak (in the sense of magnitude) of the current modeling residual at each stage. This geometric property is graphically illustrated in a simple one-dimensional modeling problem. Our method also has advantages over the radial basis function network training methods based on clustering (e.g. [12]–[14]). In these clustering based learning methods, the number of clusters or the model size must be learned by other means, for example, via cross-validation [15],[16]. Moreover, the regressor kernel variances also need to be decided using some other appropriate techniques.

II. METHOD

Consider the problem of fitting the \( N \) pairs of training data \( \{x_{i}, y_{i}\}_{i=1}^{N} \) with the regression model

\[
\hat{y}(x) = \sum_{i=1}^{M} w_{i} g_{i}(x) \tag{1}
\]

where \( x \) is the \( m \)-dimensional input variable; \( w_{i}, 1 \leq i \leq M \), denote the model weights; \( M \) is the number of regressors; and \( g_{i}(\bullet), 1 \leq i \leq M \), denote the regressors. We allow the regressor to be chosen as the generalized Gaussian kernel function

\[
g_{i}(x) = G(x; \mu_{i}, \Sigma_{i}) \tag{2}
\]

where \( \mu_{k} \) is the \( k \)th kernel center or mean vector and the covariance matrix \( \Sigma_{i} \) is diagonal. We will adopt an incremental approach to build up the regression model (1) by appending regressors one by one. Let us first introduce the following notation

\[
\begin{align*}
\hat{y}_{i}^{(0)} & = y_{i} \\
\hat{y}_{i}^{(k)} & = y_{i}^{(k-1)} - w_{k} g_{k}(x_{i}) \\
& 1 \leq i \leq N
\end{align*} \tag{3}
\]

Obviously, \( y_{i}^{(k)} \) is the modeling error at \( x_{i} \) after the \( k \)th regressor has been fitted and \( y_{i}^{(0)} \) is simply the desired output for the input \( x_{i} \). Next define the mean square error (MSE) for the \( k \)-term regression model over the training data as

\[
\text{MSE}_{k} = \frac{1}{N} \sum_{i=1}^{N} \left(y_{i}^{(k)}\right)^{2} = \frac{1}{N} \sum_{i=1}^{N} \left(y_{i} - \sum_{j=1}^{k} w_{j} g_{j}(x_{i})\right)^{2} \tag{4}
\]

The incremental modeling process is terminated when \( \text{MSE}_{k} < \xi \), where \( \xi \) is a preset modeling accuracy. The termination of the model construction process can alternatively be decided by cross-validation [15],[16], and other termination criteria include the Akaike information criterion [17], the optimal experimental design criteria [9] and the leave-one-out generalization criterion [10].

At the \( k \)th stage of modeling, the regressor \( g_{k}(x) \) is fitted to the training data set \( \{x_{i}, y_{i}^{(k-1)}\}_{i=1}^{N} \) by tuning its mean vector \( \mu_{k} \) and diagonal covariance matrix \( \Sigma_{k} \). The correlation function between the regressor and the training data set
as given by
\[
C_k(\mu_k, \Sigma_k) = \frac{\sum_{i=1}^{N} g_k(x_i) y_i{(k-1)}}{\sqrt{\sum_{i=1}^{N} g_k^2(x_i) \sum_{i=1}^{N} (y_i{(k-1)})^2}} \tag{5}
\]
defines the similarity between \(g_k(x)\) and \(\{x_i, y_i{(k-1)}\}_{i=1}^{N}\). This correlation criterion can be used to position and shape a regressor. That is, \(\mu_k\) and \(\Sigma_k\) of the \(k\)th regressor are chosen to maximize \(|C_k(\mu_k, \Sigma_k)|\). After the regressor positioning and shaping, the corresponding weight is calculated by the usual least squares solution
\[
w_k = \frac{\sum_{i=1}^{N} y_i{(k-1)} g_k(x_i)}{\sum_{i=1}^{N} g_k^2(x_i)} \tag{6}
\]
Selecting regressors by maximizing \(|C_k(\mu_k, \Sigma_k)|\) is identical to incrementally minimizing the modeling MSE (4). Substituting (3) into (4) with \(w_k\) given by (6) yields
\[
\text{MSE}_k = \left( \frac{1}{N} \sum_{i=1}^{N} \left( y_i{(k-1)} \right)^2 \right) \left( 1 - C_k^2(\mu_k, \Sigma_k) \right) \tag{7}
\]
Clearly maximizing \(|C_k(\mu_k, \Sigma_k)|\) is equivalent to minimizing MSE\(_k\) with respect to \(\mu_k\) and \(\Sigma_k\). An important technique to alleviate over-fitting and improve robustness of the solution is to apply regularization [6]-[10]. The zero-order correlation criterion can be used to position and shape a regresor vector \(\mu_k\), \(\Sigma_k\) with the associated weighting \(\lambda\) and a maximum number of iterations \(J_k\) are chosen empirically.

The optimization for determining \(\mu_k\) and \(\Sigma_k\) can be performed with guided random search methods, such as the genetic algorithm [18],[19] and adaptive simulated annealing [20],[21]. However, we perform this optimization by a simple search which is re-enforced by boosting [22]-[24]. Let the vector \(v_k\) contain the mean vector \(\mu_k\) and the diagonal covariance matrix \(\Sigma_k\). Given the training data \(\{x_i, y_i{(k-1)}\}_{i=1}^{N}\), the basic boosting search algorithm is summarized:

\textbf{Initialization}: Set iteration index \(t = 0\), give the \(\varepsilon\) randomly chosen initial values for \(v_k, y_k{(0)}(t), y_k{(1)}(t), \ldots, y_k{(s)}(t)\), with the associated weighting \(\delta_j(t) = \frac{1}{J_k}\) for \(1 \leq j \leq s\), and specify a small positive value \(\xi_\varepsilon\) for terminating the search and a maximum number of iterations \(MT\).

\textbf{Step I: Boosting}
1. Calculate the loss of each point, namely \(\text{cost}_j = 1 - |C_k(u_k{(j)}(t))|, 1 \leq j \leq s\)
2. Find \(u_k^{\text{est}}(t) = \arg\min \{\text{cost}_j, 1 \leq j \leq s\}\) and \(u_k^{\text{cor}}(t) = \arg\max \{\text{cost}_j, 1 \leq j \leq s\}\)
3. Normalize the loss
\[
\text{loss}_j = \frac{\text{cost}_j}{\sum_{j=1}^{s} \text{cost}_j}, 1 \leq j \leq s
\]
4. Compute a weighting factor \(\beta_j\) according to
\[
\beta_j = \frac{\text{loss}_j}{\sum_{j=1}^{s} \text{loss}_j}, 1 \leq j \leq s
\]
5. For \(j = 1, \ldots, s\), update the distribution weightings
\[
\delta_j(t+1) = \begin{cases} \frac{\delta_j(t)}{\beta_j^\text{loss}_j} & \text{for } \beta_j \leq 1, \\ \frac{\delta_j(t)}{\beta_j^1 - \text{loss}_j} & \text{for } \beta_j > 1, \end{cases}
\]
6. Normalize the weighting vector
\[
\delta_j(t+1) = \frac{\delta_j(t+1)}{\sum_{j=1}^{s} \delta_j(t+1)}, 1 \leq j \leq s
\]

\textbf{Step 2: Parameter updating}
1. Construct the \((s+1)\)th point using the formula
\[
u_k{(s+1)}(t) = \sum_{i=1}^{s} \delta_i(t+1) u_k{(i)}(t)
\]
2. Construct the \((s+2)\)th point using the formula
\[
u_k{(s+2)}(t) = u_k^{\text{cor}}(t) - u_k^{\text{est}}(t) - u_k{(s+1)}(t)
\]
3. Choose a better point (smaller loss value) from \(u_k{(s+1)}(t)\) and \(u_k{(s+2)}(t)\) to replace \(u_k^{\text{cor}}(t)\)

Set \(t = t+1\) and repeat from \textbf{Step I} until \(|u_k{(s+1)}(t) - u_k{(s+1)}(t-1)| < \xi_\varepsilon\) or \(MT\) iterations have been reached. Then choose the \(k\)th regressor \(u_k = u_k^{\text{est}}(t)\)

The above basic boosting search algorithm performs a guided random search and solution obtained may depend on the initial choice of the population. To derive a robust algorithm that ensures a stable solution, we augment it into the following repeated boosting search algorithm.

\textbf{Initialization}: Specify a maximum repeating times \(M_R\) and a small positive number \(\xi_\varepsilon\) for stopping the search.

\textbf{First generation}: Randomly choose the \(s\) number of initial population \(u_k^{(1)}, u_k^{(2)}, \ldots, u_k^{(s)}\), and call the boosting search algorithm to obtain a solution \(u_k^{(s+1)}(0)\)

\textbf{Repeat loop}: For \(l = 1 : M_R\)

Set \(u_k = u_k^{(s+1)}(l-1)\), and randomly generate the other \(s-1\) points \(u_k^{(i)}\) for \(2 \leq i \leq s\)

\textbf{Calling the boosting search algorithm to obtain a solution}

\(u_k^{(s)}(l)\)

If \(|u_k^{(s)}(l) - u_k^{(s)}(l-1)| < \xi_\varepsilon\), exit loop
End for

Choose the \(k\)th regressor as \(u_k = u_k^{(s)}(l)\)

The algorithmic parameters that need to be chosen appropriately are the population size \(s\), termination criterion \(\xi_\varepsilon\) and maximum number of iterations \(MT\) in the boosting search as well as the maximum number of repeating times \(M_R\) and the stopping criterion \(\xi_\varepsilon\) for the repeating loop. To simplify the algorithm tuning, we can simply fix \(M_R\) and \(M_R\) without the need to specify \(\xi_\varepsilon\) and \(\xi_\varepsilon\). In the following modeling experiments, the value of \(s, M_T, M_R\) were chosen empirically to ensure that the incremental modeling procedure produced consistent final models with the same levels of modeling accuracy and model sparsity for different runs. The stopping threshold \(\xi_\varepsilon\) for the incremental modeling procedure should ideally be set to a value slightly larger than the system noise variance. Since the system noise level is generally unknown \textit{a priori}, an appropriate value for \(\xi_\varepsilon\) has to be learned during the modeling process. Alternative, the Akaike information criterion [17] and the optimal experimental design criteria [9] can be employed to terminate the model construction procedure without the need to specify a modeling accuracy \(\xi_\varepsilon\).
III. EXPERIMENTAL RESULTS

Two examples were used to illustrate the proposed sparse modeling approach. The first example was a one-dimensional simulated data set and was chosen to demonstrate graphically the motivation and desired property of the incremental regression procedure using the correlation criterion. The second example was a real-data set. 

**Example 1.** The 500 points of training data were generated from 

\[ y(x) = 0.1x + \sin \frac{x}{x} + \sin 0.5x + \epsilon \]

with equal-spaced \( x \in [-10, 10] \), where \( \epsilon \) was a Gaussian white noise with zero mean and variance 0.01. With a population size \( s = 5 \), the maximum number of iterations \( M_I = 20 \) and the maximum repeating times \( M_R = 10 \) together with the modeling accuracy set to \( \xi = 0.012 \), the incremental modeling consistently produced models of 6 Gaussian regressors with the same \text{MSE}_\text{A} = 0.011 for a large number of different runs. We also used the Akaike information criterion [17] and the optimal experimental design criteria [9] to stop the selection procedure, rather than specifying the modeling accuracy \( \xi \), and the results obtained are identical. The construction process in a typical run is illustrated graphically in Fig. 1 (a)–(f), where the effectiveness of regressor tuning based on the correlation criterion is clearly demonstrated. In Fig. 2 (a), the model output from the constructed 6-term model is superimposed on the noisy training data, and the final modeling errors are shown in Fig. 2 (b).

**Example 2.** This example constructed a model representing the relationship between the fuel rack position (input \( u(t) \)) and the engine speed (output \( y(t) \)) for a Leyland TL11 turbocharged, direct injection diesel engine operated at a low engine speed. Detailed system description and experimental setup can be found in [25]. The data set contained 410 samples. The first 210 data points were used in training and the last 200 points in model validation. The training data set was constructed with \( y_i = y(i) \) and \( x_i = [y(i-1) \ u(i-1) \ u(i-2)]^T \) for \( i = 3, 4, \cdots, 210 \). We used the proposed approach to fit a generalized Gaussian regression model to this data set. With \( s = 37 \), \( M_I = 60 \) and \( M_R = 20 \) together with \( \xi = 0.00055 \), the incremental modeling produced in repeated runs consistent models of 9 Gaussian regressors with the MSE values of 0.00053 and 0.00050 over the training and testing sets, respectively. Fig. 3 (a) depicts the model prediction \( \hat{y}(t) \) for a typical 9-term model obtained, in comparison with the system output \( y(t) \). The corresponding model prediction error \( \epsilon(t) = y(t) - \hat{y}(t) \) is shown in Fig. 3 (b). We also ran the experiments using the Akaike information and optimal experimental design criteria to stop the modeling process, and the results obtained were similar to those obtained with given the modeling accuracy of \( \xi = 0.00055 \).

Various existing state-of-art kernel modeling techniques had been used to fit this data set in [9],[10]. These kernel modeling techniques can only choose the kernel mean vectors from the training input data points and use a single fixed common variance for all the regressors. The best Gaussian kernel model with an optimal single common variance of \( \sigma^2 = 1.69 \) obtained by one of the existing state-of-art kernel modeling techniques required at least 20 model regressors to achieve the same modeling accuracy (see [10]). In comparison, the proposed modeling approach resulted in a much sparser 9-term generalized Gaussian kernel model.

IV. CONCLUSIONS

An incremental modeling technique has been presented to construct sparse generalized Gaussian regression models. The proposed technique can tune the mean vector and diagonal covariance matrix of individual Gaussian regressor to best fit the training data incrementally based on the correlation between the regressor and the training data. A simple boosting search algorithm has been adopted for regressor tuning at each modeling stage. Experimental results using this construction technique have demonstrated that it offers a viable alternative to the existing state-of-art kernel modeling methods for constructing parsimonious regression models.
REFERENCES


Fig. 2. Incremental modeling results for the simple function fitting problem: in (a) outputs $y_1$ of the final 6-term model are superimposed on the noisy training data $y_i$, and (b) shows the final modeling errors.

Fig. 3. The engine data set: (a) model output $y(t)$ (dashed) superimposed on system output $y_i(t)$ (solid), and (b) model prediction error $e(t) = y(t) - y_i(t)$.