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A novel high level canonical piecewise linear model based on the simplicial partition and its application

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ABSTRACT

The piecewise linear (PWL) model has attracted more and more attention in recent research because it can handle complex nonlinearity while maintaining linearity in local regions. A large number of compact representations for PWL modeling have been introduced, such as hinging hyperplanes and its generalized version. However, the existing methods usually give rise to many and complex subregions, which is an issue known as "curse of partitions", and hampered practical applications of PWL models. In this paper, a novel high level canonical PWL model is presented to tackle the curse of partitions. In more detail, an improved simplicial partition strategy with alterable intervals is proposed to improve the model representation capability. The proposed PWL model guarantees an unchangeable topology during training and thus a limited number of subregions after training. Several numerical experiments, and a simulated chemical process, are used to demonstrate the effectiveness of the proposed model.

1. Introduction

In the field of data-driven modeling, a large variety of models are available, such as artificial neural networks (ANN), principal component analysis (PCA), partial least squares (PLS), supporting vector machine (SVM), piecewise linear (PWL) model and so on; see e.g. [1,2] for comprehensive reviews of this area. However, linear models, such as PCA and PLS, are not suitable for high nonlinear systems that are often seen in the real world. To this end, nonlinear models are needed, and among those, PWL model is an attractive option [3]. The main feature of the PWL model is that it is locally linear in subregions while globally nonlinear, which is important when the model is subsequently used for the purpose of e.g. optimization. As such, practical applications of PWL have been widely reported in recent years [4–8].

Since Chua and Kang [9] introduced the first compact PWL representation model, a series of compact PWL representations were reported, and landmark results are provided by Breiman [10], Lin et al. [11], Julián et al. [12], Wang and Sun [13], and Xu et al. [14]. The main advantage of compact representations of PWL is its simple and compact model formulation. However, lots of unexpected subregions are generated after model training. To illustrate this point, take the widely used hinging hyperplane (HH) model and the test function provided by Cherkassky et al. [15] as an example. The initial partition and the one after training are shown in Fig. 1. Clearly, lots of unpredicted and unexpected subregions emerge after training, and it will be worse when a large numbers of partitions are initialized. This is the so-called "curse of partitions". The model with a complex partition is inconvenient for applications.

To avoid it, Huang et al. [16] introduced a vertex adjusting algorithm to maintain the partition topology during training. Without any doubt, this can avoid the emergence of excessive unexpected partitions. However, the final fitting accuracy is largely dominated by the initial partition.

The high level canonical piecewise linear model introduced by Julián [12] can effectively avoid the curse of partitions, but the main drawback is the insufficient representation capability. To improve the representation capability and approximating ability, a novel high-level canonical PWL model is proposed in this paper. Compared with the work by Julián [12], the main improvement is that the lattice divisions of the domain are alterable. The proposed model largely improves the representation capability by introducing alterable intervals for the simplicial partition strategy. To realize the proposed simplicial

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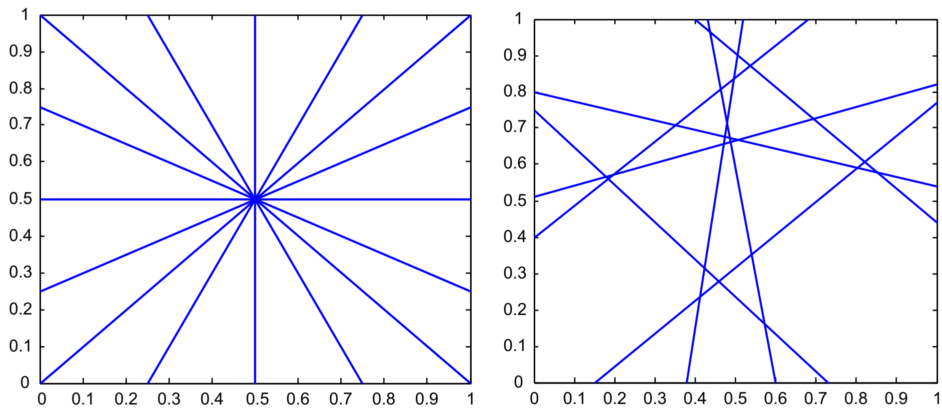

Fig. 1. Initial partition and partition after model training.

partition strategy, a special model construction method with handpicked basis functions is addressed. Then, the proposed PWL model is adopted in the scheduling model of a typical hydroupgrading processing unit, diesel hydrotreater.

This paper is organized as follows. In Section 2, the simplicial partition strategy and the corresponding handpicked basis functions are investigated, and an alternative parameters training algorithm is proposed. Numerical experiments are carried out in Section 3. Section 4 provides an application case considering the yield changes with operating conditions of a typical hydroupgrading processing unit, diesel hydrotreater, based on the famous simulation software Petro-SIM. Section 5 ends the paper with a brief conclusion.

2. A novel high level canonical PWL based on a simplicial partition with alterable intervals

This section first discusses how to partition the domain into subregions to improve the representation capability, within each of which a linear model can then be developed. Then, a parameters training algorithm is introduced. The main idea and results can also be found in [18]. In this paper, a two-dimension model is considered, partly because this is required by the particular refinery under study and partly because of the simplicity in presentation. In principle, a recursive construction method could be used to extend the two-dimensional partition to higher dimensions, which may significantly increase the model complexity and computation. High dimensional partitioning strategies will be a topic for further research.

2.1. Simplicial partition and its basis functions

The concept of simplicial partition strategy is illustrated by using a two-dimensional case. Suppose that the domain of a to-be-fitted function is $[0, a] \times [0, b]$, and the numbers of grids are $I \times J$, determined by a cross-validation procedure. The simplicial partition refers to the shaded triangular regions in Fig. 2, denoted $\Omega_{i,j} = \cup_{k=1}^{8} \Omega_{i,j,k}$, with the boundary $[\xi_i, \xi_{i+1}] \times [\zeta_j, \zeta_{j+1}]$. Such a partition strategy is the trade-off between representation capability and partition complexity. It has been demonstrated that the simpler lattice partition is inadequate in its representation capability [17], while others make the partition configuration complex, and are difficult for subsequent use.

In the following, we introduce a model construction method to realize the proposed partition strategy, shown in Fig. 2, using mathematical functions.

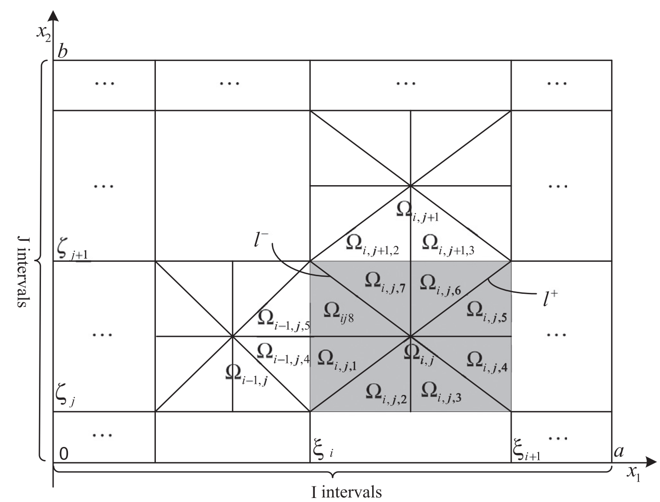

Fig. 2. Simplicial partition.

Firstly, we introduce the generating function defined by Julián [12],

$$\gamma_\psi(f_i, f_j) = \frac{1}{4}\Big\{\psi(\psi(-f_i) + f_j) - \psi(-f_i + \psi(f_j)) + \psi(-f_i) + \psi(f_j) - \psi(-f_i + f_j)\Big\} \tag{1}$$

where $\psi(z) = |z|$. In order to simplify the notation, $\gamma_\psi(f_i, f_j)(\cdot)$ is abbreviated to $\gamma(f_i, f_j)$. Clearly, the generating function follows that

$$\gamma(f_i, f_j) = \begin{cases} f_i & \text{if } 0 \le f_i \le f_j \\ f_j & \text{if } 0 \le f_j \le f_i \\ 0 & \text{if } f_i \le 0 \text{ or } f_j \le 0 \end{cases} \tag{2}$$

Define $\gamma^k(f_1, \ldots, f_k) = \gamma(f_1, \gamma^{k-1}(f_2, \ldots, f_k))$, and $\gamma^0(f_i) = f_i$, for any function f_i. For more detailed properties of the generating function refer to [12].

Then, we use the generating functions to formulate the subregions.

Firstly, take the lines l^+ and l^- into consideration, which can be represented by

$$l^+ : (x_1 - \xi_i)(\zeta_{j+1} - \zeta_j) - (x_2 - \zeta_j)(\xi_{i+1} - \xi_i) = 0$$
$$\text{or } (\xi_{i+1} - x_1)(\zeta_{j+1} - \zeta_j) - (\zeta_{j+1} - x_2)(\xi_{i+1} - \xi_i) = 0$$
$$l^- : (x_1 - \xi_i)(\zeta_{j+1} - \zeta_j) - (\zeta_{j+1} - x_2)(\xi_{i+1} - \xi_i) = 0$$
$$\text{or } (\xi_{i+1} - x_1)(\zeta_{j+1} - \zeta_j) - (x_2 - \zeta_j)(\xi_{i+1} - \xi_i) = 0$$