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Identification of a Pilot Scale Distillation Column: A Kernel Based Approach

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Abstract: This paper describes the identification of a binary distillation column with *Least-Squares Support Vector Machines (LS-SVM)*. It is our intention to investigate whether a kernel based model, particularly an LS-SVM, can be used for the simulation of the top and bottom temperature of a binary distillation column. Furthermore, we compare the latter model with standard linear models by means of mean-squared error (MSE). It will be demonstrated that this nonlinear model class achieves higher performances in MSE than linear models in the presence of nonlinear distortions. When the system is close to linear, the performance of the LS-SVM is only slightly better than the linear models.

Keywords: Chemical Industry; Distillation columns; kernel based system identification

1. INTRODUCTION

In a world where economic and environmental issues become more and more important, efficient knowledge of the behavior of a process has become indispensable. Mathematical models are heavily exploited for the predicting of process behaviour, e.g., in view process monitoring and control. In the case of control, prediction and simulation is mostly done by linear models (Qin and Badgwell, 2003). In the academic world, however, an evolution towards nonlinear models can be observed. Both linear and nonlinear models can be built on mechanistic knowledge (white-box models) or available input-output data (black-box models). As methods of the latter class can generally be employed flexibly and without a large effort, these (linear) black-box are often preferred in industrial practice. In contrast to linear systems where black-box system identification techniques are well understood and described (Ljung, 1999), for nonlinear systems a variety of possible model structures and techniques exists, e.g., neural networks, wavelets, fuzzy models and Least Squares Support Vector Machines. In this paper we focus on the applicability of LS-SVMs for black-box system identification of a pilot scale binary distillation column. As most of industrial process control applications use linear models, the LS-SVM models are compared to standard linear techniques as transfer function models, subspace state-space models and the Box-Jenkins type models. This paper is structured as follows. The next section focuses on the model structure of an LS-SVM. Section 3 introduces the binary distillation column. Section 4 presents the identification procedure. In Section 5 the results are presented. Finally, Section 6 summarises the main conclusions.

2. LEAST SQUARES SUPPORT VECTOR MACHINES

The standard framework for LS-SVM is based on a primal-dual formulation. Given a training data set $\mathcal{D}_n = \{(u_k, y_k) : u_k \in \mathbb{R}^d, y_k \in \mathbb{R}; k = 1, \dots n\}$ of size n:

$$y_k = m(u_k) + \epsilon_k, \qquad k = 1, \dots, n, \tag{1}$$

where $\epsilon_k \in \mathbb{R}$ are assumed to be independent and identically distributed zero mean random errors with finite variance. The optimization problem of finding the vector w and $b \in \mathbb{R}$ for regression can be formulated as follows (Suykens et al., 2002):

$$\begin{aligned} \min_{w,b,e} \mathcal{J}(w, e) &= \tfrac{1}{2} w^T w + \tfrac{\gamma}{2} \sum_{k=1}^{n} e_k^2 \\ \text{s.t.} \quad y_k &= w^T \varphi(u_k) + b + e_k, \quad k = 1, \dots, n, \end{aligned} \tag{2}$$

where $\varphi : \mathbb{R}^d \to \mathbb{R}^{n_h}$ is the feature map to the high dimensional feature space (Vapnik, 1999), unknowns $w, b \in \mathbb{R}$ and residual e. However, we do not need to evaluate w and $\varphi(\cdot)$ explicitly. By using Lagrange multipliers for the optimization problem (2):

$$\begin{aligned} \mathcal{L}(w, b, e; \alpha) = \frac{1}{2} w^T w + \frac{\gamma}{2} \sum_{k=1}^{n} e_k^2 \\ - \sum_{k=1}^{n} \alpha_k \{ w^T \varphi(u_k) + b + e_k - y_k \}, \end{aligned}$$

where α_k are the Lagrange multipliers, the Karush-Kuhn-Tucker (KKT) conditions for optimality are given by $\frac{\partial \mathcal{L}}{\partial w} = \frac{\partial \mathcal{L}}{\partial b} = \frac{\partial \mathcal{L}}{\partial e_k} = \frac{\partial \mathcal{L}}{\partial \alpha_k} = 0$. After elimination of the variables w and e, the solution is given by the linear system (3):

$$\left(\begin{array}{c|c} 0 & 1_n^T \\ \hline 1_n & \Omega + \frac{1}{\gamma} I_n \end{array}\right) \left(\frac{b}{\alpha}\right) = \left(\frac{0}{Y}\right), \tag{3}$$

with $Y = (y_1, \dots, y_n)^T$, $1_n = (1, \dots, 1)^T$, $\alpha = (\alpha_1, \dots, \alpha_n)^T$ and $\Omega_{kl} = \varphi(u_k)^T \varphi(u_l) = K(u_k, u_l)$, with $K(u_k, u_l)$ a positive definite kernel $(k, l = 1, \dots, n)$. According to Mercer's theorem (Mercer, 1909), the resulting LS-SVM model for new inputs becomes:

$$\hat{m}(u^\star) = \sum_{k=1}^{n} \hat{\alpha}_k K(u^\star, u_k) + \hat{b}, \tag{4}$$

where K is any positive definite kernel. In this paper we choose $K = \exp(-\|u_k - u_l\|_2^2/\sigma^2)$. The training of the LS-SVM model involves an optimal selection of the tuning parameters e.g. σ and γ, which are tuned via 10-fold cross-validation.

3. DISTILLATION COLUMN SET-UP

The experimental set-up involves a computer-controlled packed distillation column (see Fig. 1 and 2). The column is about 6 m high and has an internal diameter of 6 cm. The column works under atmospheric conditions and contains three sections of about 1.5 m with Sulzer CY packing (Sulzer, Winterthur) responsible for the separation. This packing has a contact surface of 700 m^2/m^3 and each meter packing is equivalent to 3 theoretical trays. The feed stream containing a mixture of methanol and isopropanol is fed into the column between packed sections 2 and 3. The temperature of the feed can be adjusted by an electric heater of maximum 250 W. At the bottom of the column a reboiler is present containing two electric heaters of maximum 3000 W each. In the reboiler, a part of the liquid is vaporised while the rest is extracted as bottom stream. At the column top a total condenser allows the condensation of the entire overhead vapour stream, which is then collected in a reflux drum. A part of the condensed liquid is fed back to the column as reflux, while the remainder leaves the column as the distillate stream.

In this set-up the following four variables can be manipulated: the reboiler duty Qr (W), the feed rate Fv (g/min), the duty of the feed heater Qv (W) and the reflux flow rate Fr (g/min). The distillate flow Fd (g/min) is adjusted to maintain a constant reflux drum level. Measurements are available for the reflux flow rate Fr, the distillate flow rate Fd, the feed flow rate Fv and nine temperatures, i.e., the temperature at the top of the column Tt, the temperatures in the center of every packing section (i.e. $Ts1$, $Ts2$ and $Ts3$, respectively), the temperature $Tv1$ between section 1 and 2, the temperature $Tv2$ between section 2 and 3, the temperature Tb in the reboiler of the column, and the temperatures of the feed before and after heating (i.e. $Tv0$ and $Tv2$, respectively). All temperatures are measured in degrees Celsius. The actuators and sensors are connected to a Compact Fieldpoint (National Instruments, Austin) with a controller interface cFP-2100 and I/O modules cFP-AIO-610, cFP-AIO-610 and cFP-AI-110. A Labview (National Instruments, Austin) program has been developed to control the actuators and to register the variables.

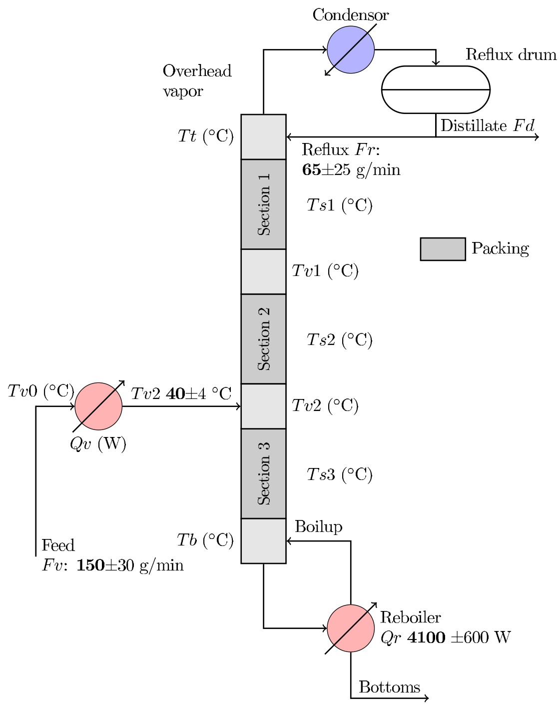

Fig. 1. Diagram of the pilot scale distillation column. Nominal set-points are printed in bold and are followed by the maximum admissible deviations.

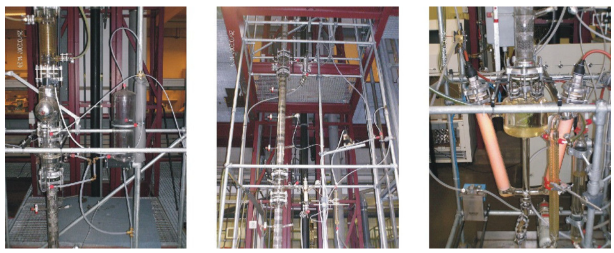

Fig. 2. Pictures of the pilot-scale distillation column: condenser (left), packed section and feed introduction (center), and reboiler (right).

4. MODEL IDENTIFICATION

In order to construct the LS-SVM model, the following steps are performed: (*i*) Experiment, (*ii*) Data preparation, (*iii*) Parameter estimation as described in Section 2 performed with the LS-SVMlab Toolbox (De Brabanter et al., 2010), and (*iv*) Validation. For the linear models, (*iii*) is replaced by model selection and parameter estimation performed with the Matlab System Identification Toolbox (Ljung, 2009).

4.1 Experiments

In order to generate estimation and validation data for system identification, an experiment is performed. The excitation signal is build up with Pseudo Random Binary (PRB) signals for the different manipulated variables.