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Modeling and prediction of flotation performance using support vector regression

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ABSTRACT

Continuous efforts have been made in recent year to improve the process of paper recycling, as it is of critical importance for saving the wood, water and energy resources. Flotation deinking is considered to be one of the key methods for separation of ink particles from the cellulose fibres. Attempts to model the flotation deinking process have often resulted in complex models that are difficult to implement and use. In this paper a model for prediction of flotation performance based on Support Vector Regression (SVR), is presented. Representative data samples were created in laboratory, under a variety of practical control variables for the flotation deinking process, including different reagents, pH values and flotation residence time. Predictive model was created that was trained on these data samples, and the flotation performance was assessed showing that Support Vector Regression is a promising method even when dataset used for training the model is limited.

1. Introduction

Paper production, due to its constantly increased consumption in recent years, has a huge environmental impact. The most obvious one is the overconsumption of wood resources, but it is also associated with pollution, water and energy consumption. Hence, recycling of waste paper is extremely important, as the production of recycled paper uses up to 50 % less energy compared to paper produced from trees, decreases air pollution significantly and saves 17-24 trees per each tone of produced paper (Costa et al, 2005).

One of the most important tasks in the process of paper recycling is removing the ink from wastepaper without damaging the cellulose fibres, meaning that a fibre could be reused up to seven times before being permanently disposed. As opposed to some other materials, paper can be recycled only limited numbers of times, as the fibres tend to become shorter and lose its quality with each subsequent recycling (Bajpai, 2014; Trumic et al., 2016).

There are many available techniques for wastepaper recycling, and the choice of the technology depends heavily on the type and quality of the raw material and the required quality of the final product (Carre et al, 2007). One of the most frequently used techniques for removing ink particles and other contaminants from cellulose fibers is deinking flotation. In the flotation process, air is bubbled through a low consistency paper suspension, where bubble interacts with hydrophobic ink particles, forming bubble-particles agglomerate that lifts away into the foam layer. The foam, that should ideally contain only the ink particles and other contaminants, is scraped away as a reject stream, while the accept stream should contain cellulose fibers, fillers and water (Trumic et al., 2007). However, the ideal separation is not possible, because deinking flotation is a very comlpex process which depends on different physical and chemical parameters. Although each of these parameters influences the deinking flotation independently, their mutual interdependence is also very important. The aim of this paper is prediction and modeling of separation of ink particles and cellulose

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fibres during the deinking flotation process of printed paper using Support Vector Regression (SVR). The concentration of oleic acid as the surfactant, pH value and residence time in flotation, are used as the input model parameters, where as the toner recovery in reject stream and celulose fiber recovery in accept stream are used as the output model parameters.

Predictive modeling is based on the analysis of relationships between the input variables in order to make predictions about the continuous output variables. In supervised machine learning these relationships are learned from the data, during the process that is referred to as training. The trained model can be further applied to input data parameters that were not used during the training process, enabling in this way the extraction of implicit and previously unrevealed properties about the modeled process from the data.

Only a limited number of studies reports the application of machine learning to deinking processes. Artificial Neural Networks (ANN) are used for modelling and prediction of the flotation deinking behaviour of industrial paper recycling processes (Pauck et al., 2014), while Labidi et al. (2007) propose a model for prediction of flotation efficiency of ink removal based on ANN. Verikas et al. (2000) developed a method for monitoring of ink removal based on neural network color image analysis. Laperrière and Wasik (2001) applied ANNs for modeling and simulation of pulp and paper quality characteristics. Multivariate Nonlinear Regression (MNLR), Radial Basis Function Neural Networks (RBFNN) and Recurrent Neural Networks (RNN) were employed to predict the flotation performance (Nakhaei & Irannajad, 2015). Chehreh Chelgania et al. (2018) used SVR for modeling of coal flotation. However, to the best of our knowledge, Support Vector Regression was not previously used for prediction and modeling of deinking flotation performance.

The remaining of this paper is organized as follows. In Section 2. SVR method is explained. In Section 3. obtained experimental results are presented and discussed. Concluding remarks are given in Section 4.

2. Support vector regression

Support Vector Machines (SVM) is a supervised machine learning method originally developed for solving binary classification problems. Suppose the data points are given as *N*-dimensional vectors. SVM searches for a linear classifier that separates the data into two classes such that the margin (separation) between two classes is maximal. In case the data points are two-dimensional, the separator is simply the line; for three-dimensional data points, the separator is the plane and for *N*-dimensional data vectors the separator is the (*N*-1)-dimensional hyperplane. Data points that lie closest to the margin are called support vectors.

If the data points $x_i \in R^n$ are not linearly separable in the given input space, they can be mapped into a higher-dimensional space using a transform $\varphi(x_i)$, where the separation might be possible. We introduce the kernel function related to the transform $\varphi(x_i)$ using the relation $k(x_i, x_j) = \varphi(x_i) \cdot \varphi(x_j)$ (Cortes & Vapnik, 1995). Hence, the decision boundary may be nonlinear in the original input space, but be a hyperplane in the transformed high-dimensional feature space. Some common kernel functions are linear, polynomial, radial basis function, sigmoid etc. SVM can also be used to solve regression problem. In that case it is denoted as Support Vector Regression (SVR). Regression is a predictive technique that models the relationship between a dependent variable (output) and a set of independent variables (inputs). As oposed to classification where the output variable is discrete (class label), in regression the output variable takes continuous values. Since the output is a real number, it is not possible to give an exact prediction as in classification case; hence an error ε is introduced and the loss function is defined that ignores all the errors that are situated within the error ε of the true value (Vapnik, 1995). An example of one-dimensional linear SVR is given in Figure 1.

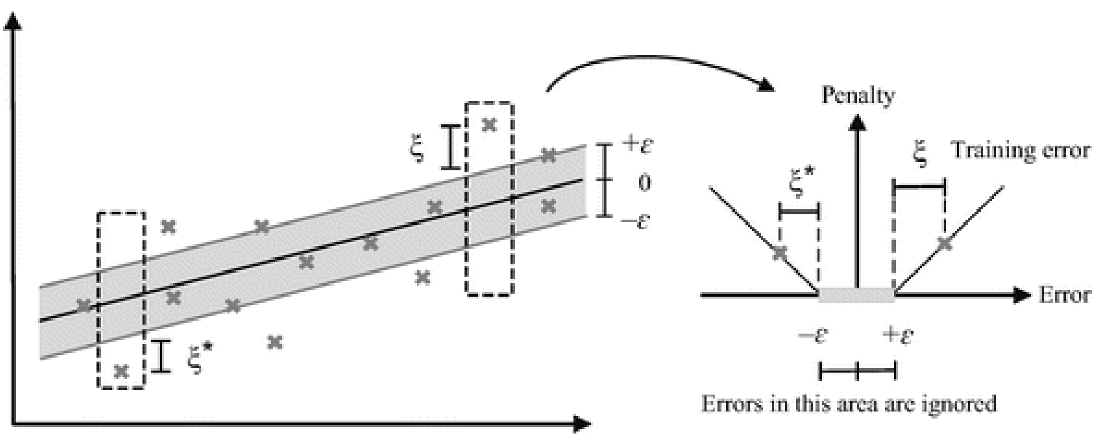

Figure 1. One-dimensional linear SVR

Let us define *N* data points used for training an SVR model $x_i \in R^n, i = 1,2,..., N$ and the target variable that needs to be predicted $y_i, i = 1,2,..., N$. The goal of SVR is to determine a function $f(x)$ that deviates from y_i by a value not greater than ε for each training data point x_i.

$$f(x) = \langle \omega, x \rangle + b; \quad \omega \in R^n, b \in R \tag{1}$$

where ω is the weight, *b* is the bias and $\langle \cdot,\cdot \rangle$ denotes the dot product. Values ω and *b* are determined from the training data by maximizing the margin $2/\|\omega\|$, or equivalently by minimizing $\frac{1}{2}\|\omega\|^2$, where the factor $\frac{1}{2}$ is used for mathematical convenience only (Vapnik et al., 1997):

$$\arg\min \frac{1}{2}\|\omega\|^2; \text{ subject to } \begin{cases} y_i - f(x_i) \le \varepsilon \\ f(x_i) - y_i \le \varepsilon \end{cases} \tag{2}$$

It is assumed that y_i exists such that for each pair $(x_i, f(x_i))$ the optimization problem is solvable with the error ε from the true value. In case there is no model that satisfies given constraints, the error tolerances ξ_i, ξ_i^* are introduced (see Figure 1) and the optimization problem becomes:

$$\arg\min \frac{1}{2}\|\omega\|^2 + C\sum_{i=1}^{N}\left(\xi_i + \xi_i^*\right); \text{ subject to } \begin{cases} y_i - f(x_i) \le \varepsilon + \xi_i \\ f(x_i) - y_i \le \varepsilon + \xi_i^* \\ \xi_i, \xi_i^* \ge 0 \end{cases} \tag{3}$$

where constant *C*>0 defines the amount of error larger than ε that is tolerated. This optimization problem can be solved using Lagrange multipliers. To obtain the dual formula, a Lagrange function is constructed from the primal function by introducing nonnegative Lagrange multipliers α_i, α_i^*, η_i, η_i^* for each training data point x_i.

$$\begin{aligned} J\left(\omega, \xi_i, \xi_i^*, \alpha_i, \alpha_i^* \eta_i, \eta_i^*\right) = \frac{1}{2}\|\omega\|^2 + C\sum_{i=1}^{N}\left(\xi_i + \xi_i^*\right) - \sum_{i=1}^{N}\left(\eta_i \xi_i + \eta_i^* \xi_i^*\right) \\ - \sum_{i=1}^{N}\alpha_i\left(\varepsilon + \xi_i - y_i + f(x_i)\right) - \sum_{i=1}^{N}\alpha_i^*\left(\varepsilon + \xi_i^* + y_i - f(x_i)\right) \end{aligned} \tag{4}$$

The solution is found by differentiating *J* with respect to $\omega, b, \xi_i, \xi_i^*$ and equating with zero, which leads to solution:

$$\begin{aligned} \omega &= \sum_{i=1}^{N}\left(\alpha_i - \alpha_i^*\right) \cdot x_i \\ b &= y_i - \langle \omega, x_i \rangle - \varepsilon,\ 0 < \alpha_i < C \\ b &= y_i - \langle \omega, x_i \rangle + \varepsilon,\ 0 < \alpha_i^* < C \end{aligned} \tag{5}$$

The function used to predict new values then becomes:

$$f(x) = \sum_{i=1}^{N}\left(\alpha_i - \alpha_i^*\right) \cdot \langle x_i, x \rangle + b \tag{6}$$

where bias b is defined in (5).

If the mapping is nonlinear the kernel functions are introduced. Suppose that each data point x_i is mapped to a higher-dimensional space $\Phi : x_i \to \varphi(x_i)$ where $k(x_i, x_j) = \varphi(x_i) \cdot \varphi(x_j)$ is the kernel function. The solution to an optimization problem for the nonlinear case becomes:

$$\begin{aligned} \omega &= \sum_{i=1}^{N}\left(\alpha_i - \alpha_i^*\right) \cdot \varphi(x_i) \\ f(x) &= \sum_{i=1}^{N}\left(\alpha_i - \alpha_i^*\right) \cdot k(x_i, x) + b \end{aligned} \tag{7}$$

3. Experimental results and discussion

Experimental specimens were obtained using white paper MAESTRO A4, 80 g/m^2 that was mechanicaly striped in paper shredder, soaked in destiled water and blended to obtain specimens of cellulose fibers, and HP LaserJet CB435A toner that was heated for 60 minutes at 100 ^oC and then mechanically grained to obtain toner specimens. Specimens of cellulose fibers and toner were further withdrawn, transferred to the Denver 2,2 litre flotation cell and floated at the condition specified below in Table 1 and Table 2.

The parameters which may have a significant effect on the deinking process, but are not used as the practical control variables and must be optimized, are summarised in Table 2.

The variables surfactant concentration (oleic acid with or without $CaCl_2$), pH (in the range 3 – 12) and flotation time (in the range 1-10 min) were used as input model parameters, where as the toner recovery in foam product (E_t) and celulose fiber recovery in sink product (E_m) were used as the output model parameters to assess flotation performance. In order to calculate Em, the float and sink products were filtered through the Buchner funnel, dried at the room temperature and weighed, while the dried froth filter pads were then heated at 550 °C in a muffle furnace to determine the ash content by x-ray fluorescence (XRF), for Et calculation.

For each experiment 75 measurings were performed, i.e. 75 pairs of input/output model parameters were created. 90 % of all data were randomly selected for training the model and the remaining 10 % were used for testing the prediction ability of the created model. The data that were used for testing were not included in the training dataset.

As a measure of performanse Mean Squared Error (MSE) was used, which defines mean squared deviation between observed and predicted value of the output parameter:

$$MSE(y, f(x)) = \frac{1}{N}\sum_{i=1}^{N}\left(y_i - f(x_i)\right)^2 \qquad (8)$$

where y_i represents the observed value of the output parameter and $f(x_i)$ is the predicted value obtained using the trained model. MSE is always nonnegative with values closer to zero defining better model.

Beside MSE, the coefficient of determination R^2 was also used as a measure of performance, defined as:

$$R^2(y, f(x)) = 1 - \frac{\sum_{i=1}^{N}\left(y_i - f(x_i)\right)^2}{\sum_{i=1}^{N}\left(y_i - \bar{y}\right)^2} \qquad (9)$$

where $\bar{y}$ denotes the mean of y. Values of R^2 closer to one define better model. While MSE is an absolute measure of fit, R^2 represents a relative measure of fit.

Table 1
Ranges of deinking parameters used as the input model variables

Process control variables	Range of process control variables
Flotation pH	3 – 12
Surfactant in flotation cell:	
Oleic acid	0.1 – 6 kg/t
Oleic acid + $CaCl_2$	0.1 – 6 kg/t + 30 kg/t
Oleic acid + $CaCl_2$	0.1 – 6 kg/t + 60 kg/t
Flotation time	1 - 10 min

Table 2
Optimization variables for flotation deinking

Optimization variables	Range of optimization variables	Adopted value
Pulping pH	7 - 10 (Dorris et al., 1994; Azevedo et al., 1999; Dorris et al., 2011; Gong, 2013.)	8
Pulping time	4 - 240 min (Behin et al., 2007; Jiang et al., 2000; Pauck et al., 2012)	120 min
Pulping temperature	35 - 60 °C (Ali et al., 1994; Dorris et al., 1994; Behin et al., 2007; Pauck et al., 2014)	45 °C
Pulping consistency	5 - 18 wt % (Liphard et al., 1993; Behin et al., 2007; Jiang et al., 2000)	5 wt %
Flotation temperature	20 - 45 °C (Dorris et al., 1994; Luo et al., 2003; Pathak et al., 2011; Pauck et al., 2014)	20 °C
Flotation consistency	0,7 - 1,5 % (Azevedo et al., 1999; Labidi et al., 2007; Pathak et al., 2011; Dorris et al., 2011; Pauck et al., 2012)	1 wt %
Agitation speed	1000 - 1400 rpm (Dorris et al., 1994; Pelach Serra, 1997; Azevedo et al., 1999; Labidi et al., 2007; Pathak et al., 2011)	1100 rpm
Airflow rate	225 - 775 l/h (Pelach Serra, 1997; Labidi et al., 2007)	260 l/h

SVR was implemented using LIBSVM library (Chang et al., 2011) with radial kernel function:

$$k\langle x_i, x\rangle = \exp\left(-\gamma\|x_i - x\|^2\right),\ \gamma > 0 \qquad (10)$$

where the optimal coefficients γ and C are determined using grid search.

Tables 3-5 present results of SVR prediction of the toner recovery in foam product (E_t) and celulose fiber recovery in sink product (E_m) when oleic acid, oleic acid with addition of $CaCl_2$, respectively, were used as surfactants. High values of coefficient of determination for E_m confirm the predictive capability of SVR in all three cases, with $R^2 = 0.96$, $R^2 = 0.94$ and $R^2 = 0.97$ for differents surfactants, as listed in Tables 3-5. On the other hand, prediction of E_t leads to lower $R^2<0.9$, indicating that additional training data is necessary for creating models with higher predictive performance.

Table 3
MSE and R^2 when oleic acid was used as surfactant

Surfactant	Oleic acid	
	Em	Et
MSE	2.27	207.63
R^2	0.96	0.85

Table 4
MSE and R^2 when oleic acid + 30 kg/t $CaCl_2$ was used as surfactant

Surfactant	Oleic acid + $CaCl_2$	
	Em	Et
MSE	5.38	52.59
R^2	0.94	0.87

Table 5
MSE and R^2 when oleic acid + 60 kg/t $CaCl_2$ was used as surfactant

Surfactant	Oleic acid + $CaCl_2$	
	Em	Et
MSE	1.42	106.03
R^2	0.97	0.72

4. Conclusion

The paper presents a machine learning based approach for modeling and prediction of separation of toner particles and cellulose fibers in printed paper recycling using flotation deinking. Support Vector Regression was chosen as a method for prediction. Although dataset used for this task was limited (only 75 samples for both training and testing), the obtained result indicate that SVR is able to discover nonlinear relationship between input flotation parameters and output flotation performance measures. SVR is a promising method and suggests that even a smaller dataset can be used for training the model, which is able to generalize for unseen test data.

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Modelovanje i predikcija performansi flotacije korišćenjem metode potpornih vektora za regresiju

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I Z V O D

Poslednjih godina vrše se značajna ulaganja u poboljšanje procesa reciklaže papira kako bi se uticalo na očuvanje šumskih, vodnih i energetskih resursa. Flotacija predstavlja najznačajniji postupak za separaciju čestica tonera od vlakana celuloze iz suspenzije papira. Modelovanje procesa flotacije je vrlo složeno, a dobijeni modeli su često komplikovani za implementaciju i upotrebu. U ovom radu predstavljen je model za predikciju performansi procesa flotacije koji je zasnovan na upotrebi metode potpornih vektora za regresiju (SVR). Reprezentativni uzorci za učenje modela dobijeni su u laboratorijskim uslovima, ispitivanjem uticaja različitih promenljivih kojima se kontroliše proces flotacije, poput tipa i koncentracije surfakanta, pH vrednosti i vremena flotiranja. Dobijeni rezultati potvrđuju da se metod potpornih vektora za regresiju može uspešno koristiti za predikciju performansi procesa flotacije čak i kada je skup podataka za učenje modela ograničen.