Variable selection in censored kernel regression[†]

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Abstract

For censored regression, it is often the case that some input variables are not important, while some input variables are more important than others. We propose a novel algorithm for selecting such important input variables for censored kernel regression, which is based on the penalized regression with the weighted quadratic loss function for the censored data, where the weight is computed from the empirical survival function of the censoring variable. We employ the weighted version of ANOVA decomposition kernels to choose optimal subset of important input variables. Experimental results are then presented which indicate the performance of the proposed variable selection method.

Keywords: ANOVA decomposition kernel, censored data, generalized cross validation function, kernel function, variable selection.

1. Introduction

Suykens and Vanderwalle (1999) proposed LS-SVM, which is a least squares version of support vector machine (SVM) originally introduced by Vapnik (1995, 1998). The solution is given by a linear system instead of a quadratic programming problem. The fact that LS-SVM has explicit primal-dual formulations has lots of advantages. Kernel tricks are used in SVM and LS-SVM to treat the nonlinear relation between input variables and output variable. See Cho et al. (2010), Hwang (2010a, 2010b), Shim and Lee (2009) for the reference.

The censored regression model and the least squares method to accommodate the censored data seem appealing since they are familiar and well understood. Koul et al. (1981) gave a simple least squares type estimation procedure in the censored regression model with the weighted observations and also showed the consistency and asymptotic normality of the estimator. Zhou (1992) proposed an M-estimator of the regression parameter of censored regression model based on the weights proposed by Koul et al. (1981). Orbe et al. (2003) proposed the estimation procedure of censored regression model where estimators of regression parameters and nonlinear function are obtained by minimizing the penalized weighted least squares objective function through iterative method. They also proposed the procedure

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to generate the bootstrap resamples to obtain the uncertainty measures of estimators. Jin et al. (2003) proposed the estimation procedure where regression parameter estimates of censored regression model are obtained from non-monotone estimating equations based on the weighted log-rank statistics. The estimating equations are solved through iterative method with Gehan (1965)-type estimate as the initial value. Ghosh and Ghosal (2006) proposed the estimation procedure based on a nonparametric Bayesian approach which uses a Dirichlet prior for the mixture of Weibull distribution in the censored regression model, where Markov Chain Monte Carlo method (Brooks, 1998) is used to obtain the marginal posterior distribution of regression parameters. Shim $et\ al.$ (2011) proposed a semiparametric LS-SVM for the censored data using weights which Koul $et\ al.$ (1981) proposed.

In linear regression models the stepwise regression is popular in which the selection of input variables is carried out by an automatic procedure (Draper and Smith, 1981). Many variable selection techniques for linear regression models have been extended to the context of survival models, including the best-subset selection, stepwise selection, and Bootstrap procedures (Sauerbrei and Schumacher, 1992). Recently the Lasso (least absolute shrinkage and selection operator; Tibshirani, 1997) has been proposed for Cox proportional hazards model (Cox, 1972). By shrinking some regression parameters to zero, this method provides the selection of important variables and the estimation of regression parameters simultaneously. Huang et al. (2005) proposed the regularization and variable selection approach using Lasso (Tibshirani, 1996). Hu and Rao (2010) proposed a weighted least squares method with censoring constraints and sparse penalization to fit censored regression models with highdimensional covariates. There are lots of literatures in studies of variable selection: Guyon et al. (2002), Tibshirani et al. (2002), Koo et al. (2006). Guyon et al. (2002) developed SVM with a recursive features elimination algorithm and Tibshirani et al. (2002) developed the prediction analysis of microarrays method based upon an enhancement of the simple nearest prototype classifier. Recently, Shim et al. (2009) proposed the marker genes selection by the supervised weighted kernel clustering and SVM.

In this paper we propose a variable selection method in censored kernel regression, which uses the weighted ANOVA decompostion kernel. From the quadratic programming problem we obtain weights whose magnitudes imply the importance of variables on regression. The rest of paper is organized as follows. In Section 2 we present the censored kernel regression and model selection methods. In Section 3 we propose the variable selection method using the weighted ANOVA decompostion kernel. In Section 4 we perform the numerical studies with the simulated nonlinear dataset and the partially linear real dataset. In Section 5 we give the concluding remarks.

2. Censored kernel regression

In this paper we set $x_i \in R^d$ be the input vector and t_i be the response variable (survival time) corresponding to input vector, x_i or transformation on it, where $i=1,\cdots,n$. In fact we cannot observe t_i 's but the observed variable, $y_i = \min(t_i, c_i)$ and $\delta_i = I(t_i \leq c_i)$, where $I(\cdot)$ denotes the indicator function and c_i is the censoring variable corresponding to x_i for $i=1,\cdots,n$. c_i 's are assumed to be independently distributed with unknown survival distribution functions. In most practical cases survival distribution function of c_i 's, G, is not known and needs to be estimated by the Kaplan-Meier (1958) estimator or its variation. The problem considered here is the estimation of $m(x_i)$, the regression function of the response

variable given x_i , based on $(\delta_1, y_1, x_1), \dots, (\delta_n, y_n, x_n)$. Buckley and James (1979) defined the pseudo-response variable

$$y_i^* = y_i \delta_i + E(t_i | t_i > y_i, \boldsymbol{x}_i)(1 - \delta_i). \tag{2.1}$$

They showed $E(y_i^*|\mathbf{x}_i) = E(t_i|\mathbf{x}_i)$ and proposed the iteration method to estimate the regression parameters. Koul *et al.* (1981) defined new observable responses y_i^* as $y_i^* = u_i y_i$ with

$$u_i = \frac{\delta_i}{G(y_i)},\tag{2.2}$$

and showed y_i^* has the same mean as t_i and thus follows the same linear model as t_i does. Here, \widehat{G} , the Kaplan-Meier estimates (Kaplan and Meier, 1958) of survival distribution function G of c_i 's can be obtained as,

$$\widehat{G}(y) = \begin{cases} \prod_{i: y_{(i)} \le y} \left(\frac{n-i}{n-i+1}\right)^{1-\delta_{(i)}} & \text{if } y \le y_{(n)} \\ 0 & \text{otherwise} \end{cases}$$
 (2.3)

where $(y_{(i)}, \delta_{(i)})$ is (y_i, δ_i) ordered on y_i for $i = 1, \dots, n$. Koul et al. (1981) proposed the ordinary least squares regression of y_i^* on \mathbf{x}_i . Zhou (1992) proposed the weighted least squares regression of y_i^* on \mathbf{x}_i with u_i so that $(\widehat{\boldsymbol{\beta}}, \widehat{b})$ in (2.4) can be seen as the minimizer of the objective function as follows:

$$\frac{1}{2} \sum_{i=1}^{n} u_i (y_i - \mathbf{x}_i' \boldsymbol{\beta} - b)^2.$$
 (2.4)

We consider the nonlinear regression case, in which the regression function of x_i , $m(x_i)$, can be regarded as a nonlinear function of input variables,

$$m(\mathbf{x}) = \mathbf{w}'\phi(\mathbf{x}) + b.$$

Here b is a bias term and $\mathbf{w} \in R^{d_f}$ is a weight vector corresponding to the feature mapping function $\phi(\cdot): R^d \to R^{d_f}$ which maps the input space to the higher dimensional feature space where the dimension d_f is defined in an implicit way. An inner product in feature space has an equivalent kernel function in input space, $\phi(\mathbf{x}_k)'\phi(\mathbf{x}_l) = K(\mathbf{x}_k, \mathbf{x}_l)$ (Mercer, 1909). Using kernel tricks in SVM and LS-SVM, a penalized least squares optimization problem inspired by (2.4) can be considered with a penalty parameter $\gamma > 0$ as follows:

$$\min \frac{1}{2} \alpha' K \alpha + \frac{\gamma}{2} (\mathbf{y} - K \alpha - b)' U(\mathbf{y} - K \alpha - b), \tag{2.5}$$

where $K = K(\boldsymbol{x}, \boldsymbol{x})$, U is a diagonal matrix of u_i 's and $\boldsymbol{\alpha}$ is an $n \times 1$ vector such that $m(\boldsymbol{x}) = K\boldsymbol{\alpha} + b$. The estimates of $(\boldsymbol{\alpha}, b)$ can be obtained from the linear equations which are results of differentiation of (2.5) with respect to $(\boldsymbol{\alpha}, b)$,

$$\begin{pmatrix} KUK + I/\gamma & KU1 \\ \mathbf{1}'UK & \mathbf{1}'U\mathbf{1} \end{pmatrix} \begin{pmatrix} \boldsymbol{\alpha} \\ b \end{pmatrix} = \begin{pmatrix} KU \\ \mathbf{1}'U \end{pmatrix} \boldsymbol{y}. \tag{2.6}$$

Solving the linear equation (2.6), the estimated regression function given \boldsymbol{x}_t is obtained as

$$\widehat{m}(\boldsymbol{x}_t) = K(\boldsymbol{x}_t, \boldsymbol{x})\widehat{\boldsymbol{\alpha}} + \widehat{\boldsymbol{b}}, \tag{2.7}$$

which can be seen as the linear combination of y as follows:

$$\widehat{m}(\boldsymbol{x}_t) = (K(\boldsymbol{x}_t, \boldsymbol{x}), \mathbf{1}) \begin{pmatrix} KUK + I/\gamma & KU\mathbf{1} \\ \mathbf{1}'UK & \mathbf{1}'U\mathbf{1} \end{pmatrix}^{-1} \begin{pmatrix} KU \\ \mathbf{1}'U \end{pmatrix} \boldsymbol{y}. \tag{2.8}$$

For the partially linear case where the input variables can be divided into two groups - a group, x_1 , of variables which are related to the regression function linearly and the other group, x_2 , of variables which are related to the regression function nonlinearly, we can still use (2.8) by setting $K = x_1x_1' + K(x_2, x_2)$. Then the estimated regression function given (x_{1t}, x_{2t}) is obtained as

$$\widehat{m}(\boldsymbol{x}_{1t}, \boldsymbol{x}_{2t}) = (\boldsymbol{x}_{1t}\boldsymbol{x}_1 + K(\boldsymbol{x}_{2t}, \boldsymbol{x}_2))\widehat{\boldsymbol{\alpha}} + \widehat{\boldsymbol{b}}. \tag{2.9}$$

The functional structure of censored kernel regression is characterized by hyper-parameters, the penalty parameter γ and the kernel parameters. To select the optimal values of hyper-parameters of the censored kernel regression, we define a cross validation function as follows:

$$CV(\boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^{n} u_i (y_i - \widehat{m}_i^{(-i)}(\boldsymbol{\theta}))^2,$$
 (2.10)

where $\boldsymbol{\theta}$ is the set of hyper-parameters and $\widehat{m}_i^{(-i)}(\boldsymbol{\theta})$ is the predicted value of $m(\boldsymbol{x}_i)$ obtained from data without i th observation. Since for each candidates of hyper-parameters, $\widehat{m}_i^{(-i)}(\boldsymbol{\theta})$ for $i = 1, \dots, n$, should be evaluated, selecting parameters using CV function is computationally formidable.

By leaving-out-one lemma (Kimeldorf and Wahba, 1991) and the first order Taylor expansion, we have a ordinary cross validation (OCV) function (Shim *et al.*, 2011),

$$OCV(\boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^{n} u_i \left(\frac{y_i - \widehat{m}_i(\boldsymbol{\theta})}{1 - s_{ii}/n} \right)^2, \tag{2.11}$$

where s_{ii} is the i th diagonal element of S which is the hat matrix such that

$$\widehat{\boldsymbol{m}}(\boldsymbol{\theta}) = S\boldsymbol{y} = (K, \mathbf{1}) \begin{pmatrix} KUK + \mathrm{I}/\gamma & KU\mathbf{1} \\ \mathbf{1}'UK & \mathbf{1}'U\mathbf{1} \end{pmatrix}^{-1} \begin{pmatrix} KU \\ \mathbf{1}'U \end{pmatrix} \boldsymbol{y}.$$

By replacing $(1 - s_{ii}/n)$ with 1 - trace(S)/n we have a generalized cross validation (GCV) function.

$$GCV(\boldsymbol{\theta}) = \frac{n \sum_{i=1}^{n} u_i (y_i - \widehat{m}_i(\boldsymbol{\theta}))^2}{(n - trace(S))^2}.$$
 (2.12)

3. Variable selection

The ANOVA decomposition kernels are inspired by ANOVA in Statistics, which can be seen as the sum of kernels constructed by different subsets of variables (Vapnik, 1998). The ANOVA decomposition kernel has two main advantages (Saunders *et al.*, 1998) - (i) improving predictive performance by considering the different subsets as group together like variables (ii) avoiding overfitting training data by only considering some subsets of input variables.

We assume that p is the prespecified number of input variables to be selected then the ANOVA decomposition kernel is defined as follows:

$$K_p = \sum_{k=1}^{d_p} K(\mathbf{x}_{:k}, \mathbf{x}_{:k}), \tag{3.1}$$

where $\boldsymbol{x}_{:k}$ is the $n \times p$ submatrix of \boldsymbol{x} consisting of the k th subset of $I_p = \{(k_1, \dots, k_p) | 1 \le k_1 < \dots < k_p \le d\}$ and $d_p = \begin{pmatrix} d \\ p \end{pmatrix}$ is the size of I_p .

In this paperwe modify the ANOVA decomposition kernel into the weighted version such as

$$K_A = \sum_{k=1}^{d} v_k K(\boldsymbol{x}_{.k}, \boldsymbol{x}_{.k}),$$
 (3.2)

where $\mathbf{x}_{.k}$ is the k th column of \mathbf{x} , $v_k \geq 0$, $\sum_{k=1}^{d} v_k = 1$ and v_k is a weight representing the influence of k th input variable on the response. The important input variables can be selected according to magnitude of $v_k's$ such that the input variables corresponding to p largest $v_k's$ are selected as p most important input variables.

To select the prespecified number of input variables we need to find v_k 's first. But v_k 's cannot be obtained in a step but by the iterative procedure since (α, b) contains v_k . The variable selection procedure for censored kernel regression can be carried out as follows:

- (i) With $K = K(\boldsymbol{x}, \boldsymbol{x})$ find the optimal values of hyper-parameters from (2.11) and $(\boldsymbol{\alpha}, b)$ from the linear equation (2.6).
- (ii) With $(\boldsymbol{\alpha}, b)$, find $\boldsymbol{v} = (v_1, \dots, v_d)'$ from a quadratic programming problem,

$$\min \frac{1}{2} \mathbf{v}' A' U A \mathbf{v} - (\mathbf{y}' U A - b \mathbf{1}' U A - \frac{1}{2\gamma} \boldsymbol{\alpha}' A) \mathbf{v}$$
(3.3)

subject to

$$0 \le v \le 1 \text{ and } 1'v = 1,$$

where $A = (K_A^1 \boldsymbol{\alpha}, \dots, K_A^d \boldsymbol{\alpha})$ is the $n \times d$ matrix with $K_A^k = K(\boldsymbol{x}_{.k}, \boldsymbol{x}_{.k})$. The quadratic programming problem (3.3) is obtained by expressing the following optimal problem with respect to v_k 's,

$$\min \frac{1}{2} \alpha' \mathbf{K}_A \alpha + \frac{\gamma}{2} (\mathbf{y} - \mathbf{K}_A \alpha - b\mathbf{1})' U(\mathbf{y} - \mathbf{K}_A \alpha - b\mathbf{1})$$

subject to

$$0 \le v \le 1 \text{ and } 1'v = 1.$$

- (iii) Find $(\boldsymbol{\alpha}, b)$ from (2.6) by replacing \boldsymbol{K} with \mathbf{K}_A which is updated with newly obtained v_k 's in (ii) as (3.2).
- (iv) Iterate (ii) and (iii) until $||v^{(t)} v^{(t+1)}||$ converges.

4. Numerical studies

We illustrate the performance of the proposed method for the variable selection through the simulated data sets and the real data set. We indicate the performance of the proposed method by showing weighted sums of squared residuals (Zhou, 1998).

Example 4.1 In this example we generate 200 data sets to indicate the performance of variable selection by showing that the proposed method agrees with the exhaustive search using the censored kernel regression on selection of two true important input variables. For each $i = 1, \dots, 100, x_{i1}, \dots, x_{i6}$ are generated from a uniform distribution, U(0,1) and (t,c)'s are generated as follows:

$$t_i = 1 + \exp(x_{i1} + x_{i4}) + \epsilon_{t_i}, \ c_i = 1.2 + \exp(x_{i1} + x_{i4}) + \epsilon_{c_i}, \ i = 1, \dots, 100,$$

where ϵ_{t_i} 's and ϵ_{c_i} 's are generated from normal distribution, $N(0, 0.1^2)$. From 200 data sets the average and the standard error of the censoring percentage were obtained as 8.3% and 0.2%, respectively. We consider the nonlinear censored regression as follows:

$$m(\mathbf{x}_i) = \mathbf{w}'\phi(\mathbf{x}_i) + b,$$

where $\mathbf{x}_i = (x_{1i}, x_{2i}, \cdots, x_{6i})$. For each data set, a radial basis function kernel, $K(\mathbf{x}_j, \mathbf{x}_k) = \exp(-(-1/\sigma^2)||\mathbf{x}_j - \mathbf{x}_k||^2)$, is applied to the censored kernel regression and the optimal values of hyper-parameters (γ, σ^2) are chosen from GCV function in (2.12). Table 4.1 shows the number of times selected by the proposed method as the most and the secondly most important input variables in 200 data sets. For the exhaustive search using the censored kernel regression, we use $\binom{6}{2} = 15$ sets of two input variables shown in the first column heading of Table 4.3. We divided each dataset into 15 sub-data sets according to 15 sets of response, $\delta_i = I(t_i \leq c_i)$ and two input variables such as $\{y_i, \delta_i, x_{i1}, x_{i2}\}$ $\{y_i, \delta_i, x_{i1}, x_{i3}\}$ $\{y_i, \delta_i, x_{i1}, x_{i3}\}$ $\{y_i, \delta_i, x_{i2}, x_{i6}\}$ $\{y_i, \delta_i, x_{i3}, x_{i6}\}$ $\{y_i, \delta_i, x_{i5}, x_{i6}\}$ $\{y_i,$

$$wSSR(1,2) = \sum_{i=1}^{n} u_i (y_i - \widehat{m}(x_{i1}, x_{i2}))^2,$$

where $\widehat{m}(x_{i1}, x_{i2})$ is the regression function of x_i estimated from $\{y_i, \delta_i, x_{i1}, x_{i2}\}$ $_{i=1}^{100}$. We computed the averages of 200 wSSR's for each set of two input variables, which are shown in Table 4.3. By the proposed method we obtained averages of weights representing the influence of each input variable on the response in 200 dataset, which are shown in Table 4.2. From the tables we can see that the proposed method and the exhaustive search using

the censored kernel regression agree on the variable selection of (x_1, x_4) as the two most important input variables. We also compute wSSR using six input variables for each data set, whose average and standard error are obtained as 1.4223 and 0.0197, respectively, which is a little smaller than wSSR(1,4) = 1.7462 in Table 4.3.

Table 4.1 Results of Example 4.1 by proposed method

_	rubic 1.1 iv	CD direction OI	Diampi	J 1.1 DJ	propos	oca men	iou	_
	variable (i)	1	2	3	4	5	6	-
_	first	99	2	3	88	3	5	-
	second	25	38	37	29	39	32	

Table 4.2 Results of Example 4.1 by proposed method (standard error in parenthesis)

variable (i)	1	2	3	4	5	6
:	0.2376	0.1316	0.1213	0.2409	0.1508	0.1149
weight	(0.0091)	(0.0163)	(0.0157)	(0.0095)	(0.0189)	(0.0160)

Table 4.3 Results of Example 4.1 by exhaustive search (standard error in parenthesis)

variables (i, j)	average of $wSSR$	variables (i, j)	average of $wSSR$
(1, 2)	75.6055 (0.8255)	(2, 6)	147.0063 (1.6852)
(1, 3)	75.3725 (0.7839)	(3, 4)	$75.0988 \ (0.7725)$
(1, 4)	$1.7462 \ (0.0184)$	(3, 5)	147.3635 (1.7096)
(1, 5)	75.3492 (0.7855)	(3, 6)	147.0576 (1.7475)
(1, 6)	75.6332 (0.8110)	(4, 5)	75.0860 (0.7753)
(2, 3)	147.2786 (1.7989)	(4, 6)	75.6268 (0.7578)
(2, 4)	75.6595 (0.7997)	(5, 6)	146.4083 (1.6820)
(2, 5)	147.2902 (1.7703)		

Example 4.2 In this example we apply the proposed method to a study on multiple myeloma reported by Krall *et al.* (1975). Among a total of 65 patients who were treated with alkylating agents, 48 died during the study and 17 survived. The observed survival times were measured in months. There are nine input variables, which are described in Table 4.4. We consider the nonlinear censored regression as follows:

$$m(\boldsymbol{x}_i) = \boldsymbol{w}'\phi(\boldsymbol{x}_i) + b,$$

where $\mathbf{x}_i = (x_{1i}, x_{2i}, \dots, x_{9i}) = (\text{Platelet, Frac, } \dots, \text{SCalc})$. Using the radial basis kernel the regression function can be rewritten as follows:

$$m(\boldsymbol{x}_i) = K(\boldsymbol{x}_i, \boldsymbol{x})\boldsymbol{\alpha} + b.$$

A in (3.3) becomes $A=(K_A^1\boldsymbol{\alpha},K_A^2\boldsymbol{\alpha},\cdots,K_A^9\boldsymbol{\alpha})$, where $K_A^k=K(\boldsymbol{x}_{.k},\boldsymbol{x}_{.k})$ and $\boldsymbol{x}_{.k}$ is a 65 × 1 vector of the k th input variable. A radial basis function kernel is applied in the censored kernel regression and the optimal values of hyper-parameters are chosen from GCV function in (2.12) as $(\gamma,\sigma^2)=(700,4)$. By the proposed method we obtained a weight vector representing the influence of each input variable on the response as $\boldsymbol{v}=(0,0,0,0.2747,0.4721,0,0.0077,0.2454,0)'$, which implies that the most important input variables selected are rearranged in the ascending order as Age-HGB-Protein-LogPBM. For

the exhaustive search using the censored kernel regression, we use $\binom{9}{k}$ sets of k=2,3,4 input variables, wSSR(Age, HGB), wSSR(Age, HGB, Protein), wSSR(Age, HGB, Protein, logPBM), are obtained as 0.0363, 0.005, 0.0001, respectively. We obtained wSSR with all input variables as 0.0001, which is same as wSSR(Age, HGB, Protein, logPBM) and implies that (Age, HGB, Protein, logPBM) are the most important input variables when we use the censored kernel regression.

Table 4.4 Input variables of Myeloma data reported by Krall et al. (1975)

variable	description	type
Platelet	platelets at diagnosis: 0=abnormal, 1=normal	binary
Frac	fractures at diagnosis: 0=none, 1=present	binary
logBUN	log(BUN) at diagnosis	continuous
HGB	hemoglobin at diagnosis	continuous
Age	age at diagnosis in years	continuous
logWBC	log(WBC) at diagnosis	continuous
logPBM	log(PBM) at diagnosis	continuous
Protein	proteinuria at diagnosis	continuous
SCalc	serum calcium at diagnosis	continuous

*BUN: blood urea nitrogen WBC: white blood cells in the blood

PBM: plasma cells in bone marrow

5. Conclusions

In this paper, we dealt with the variable selection method in the censored kernel regression. The weights representing the influence of input variables are obtained by minimizing the quadratic programming problem composed of the weighted ANOVA decompostion kernels. The proposed method is reliable in the point that which agree with the exhaustive search in the simulated data. Through the examples we showed that the proposed method derives the good solutions to the variable selection in the censored kernel regression.

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