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Complete List of Authors	Cui Xiong Jun Shao and Lei Wang
Corresponding Author	Jun Shao
E-mail	shao@stat.wisc.edu

CONVEX SURROGATE MINIMIZATION IN CLASSIFICATION

Cui Xiong¹, Jun Shao^{1,2} and Lei Wang³

¹*East China Normal University*, ²*University of Wisconsin-Madison*
and ³*Nankai University*

Abstract: Convex optimization is an increasingly important theme in applications. We consider the construction of a binary classification rule by minimizing the risk based on a convex loss as a surrogate to the 0-1 loss. Compared with the approach of directly estimating the conditional probability of the binary class label given a vector of covariates, our proposed convex surrogate minimization approach is computationally simpler and more efficient. We begin with a discussion of what type of convex surrogate is valid. When the conditional probability model for class label is parametric, we show that our proposed approach is either equivalent to the traditional maximum likelihood method or a substitute for computational saving. When the conditional probability model is semiparametric, we show how to apply convex surrogate minimization in conjunction with kernel weighting, which results in an asymptotically valid classification rule. Some convergence rates are established and empirical simulation results are presented.

Key words and phrases: Convex optimization, binary classification, kernel weight-

ing, 0-1 loss.

1. Introduction

In many social, economical, biological, and medical studies, it is important to classify a subject into one of two classes based on a set of covariates observed from the subject. Let $Y = 1$ and -1 be the labels of the two classes and X be the p -dimensional vector of covariates observed from the subject. In most applications, variability exists and, hence, X and Y are random. A classification rule or discriminant function is any Borel function T from the range of X to $\{1, -1\}$ such that the subject is classified to class $T(X)$ when X is observed. A natural measure to evaluate the performance of a rule T is the misclassification rate $P(Y \neq T(X))$, where $P(\cdot)$ is the probability with respect to the distribution of (Y, X) .

If the distribution of (Y, X) is known, then we can construct the optimal classification rule $T^*(X) = \text{sign}\{P(Y = 1|X) - P(Y = -1|X)\}$, where $\text{sign}(x)$ is the sign of x and $P(Y = y|X)$ is the conditional probability given X . The distribution of (Y, X) is usually unknown, and classification rules are constructed using observations from a training sample, $\{(X_1, Y_1), \dots, (X_n, Y_n)\}$, which is an independent sample identically distributed as (Y, X) . A statistical issue is how to use the training sample

to construct a classification rule that has a misclassification rate close to that of the optimal rule.

Throughout this paper we assume a model

$$P(Y = 1|X) = g(\beta_0^T X), \quad (1.1)$$

where $\beta_0 = (\beta_{01}, \dots, \beta_{0p})^T$ is an unknown p -dimensional vector, a^T denotes the transpose of a vector a , g is either a known distribution function (the parametric case) or an unspecified distribution function (the semiparametric case), and $g(0) = 1/2$ is assumed. Without loss of generality, we assume that the first component of X is 1 so β_{01} is an intercept and that $p > 1$ and $\beta_{0p} \neq 0$ so there is at least one useful non-constant covariate. Under the monotonicity condition on g and $g(0) = 1/2$, the optimal rule $T^*(X) = \text{sign}(\beta_0^T X)$.

Since we know the form of the optimal rule T^* , one way to construct a classification rule based on data from the training sample is to substitute the unknown β_0 in the optimal rule by an estimator $\hat{\beta}$ based on data $(X_1, Y_1), \dots, (X_n, Y_n)$. Although we need not worry about g in the optimal rule, whether or not g is known actually affects the estimation of β_0 . When g is known, so that model (1.1) is parametric, β_0 can be estimated using the parametric method of maximum likelihood and the estimator is asymptotically (as $n \rightarrow \infty$) normal and optimal. When both g and β_0 are

unknown, model (1.1) is referred to as the single-index model and β_0 may be estimated by the method of sliced inverse regression (SIR) proposed in Li (1991, 1992), sliced average variance estimation (SAVE) proposed by Cook and Weisberg (1991), directional regression (DR) proposed in Li and Wang (2007), and extended principal fitted components (EPFC) and likelihood acquired directions (LAD) proposed in Cook and Forzani (2009). Although we can only estimate $c\beta_0$ using these methods under the single-index model, it is enough for classification because $\text{sign}(\beta_0^T X) = \text{sign}(c\beta_0^T X)$ for any $c > 0$. These estimation-based methods, however, rely on either a correct specification of the function g in the parametric case or that $E(b^T X | \beta_0^T X)$ is linear in $\beta_0^T X$ for any p -dimensional vector b satisfied if X is elliptically symmetric (Li (1991)).

The purpose of this paper is to study a different approach for the construction of a classification rule, a method that directly minimizes an estimated misclassification rate. We focus on rules having the form $\text{sign}(\beta^T X)$ for a p -dimensional vector β (which may not be β_0 and may depend on data). Let $\ell(\alpha)$ be the 0-1 loss function that is 1 if $\alpha \leq 0$, and 0 otherwise. Then the misclassification rate of any $T(X) = \text{sign}(\beta^T X)$ is the risk under the 0-1 loss,

$$R(\beta) = E\{\ell(Y\beta^T X)\} = P(Y \neq \text{sign}(\beta^T X)). \quad (1.2)$$

The expectation and probability are with respect to the distribution of (Y, X) . Here R is a function of β as well as β_0 and g , but we omit β_0 and g for simplicity. If β is an estimator, a function of the training data $\mathcal{T}_n = \{(Y_1, X_1), \dots, (Y_n, X_n)\}$, then the expectation is taken conditional on \mathcal{T}_n , and $R(\beta)$ is a function of β_0 , g , and data \mathcal{T}_n . Given the training data \mathcal{T}_n and a fixed β , it is natural to estimate $R(\beta)$ by the sample average

$$\hat{R}(\beta) = \frac{1}{n} \sum_{i=1}^n \ell(Y_i \beta^T X_i).$$

Then, we wish to find a classification rule with a β that minimizes the estimated risk $\hat{R}(\beta)$, but such a procedure is computationally intractable (Arora et al. (1997)). It has been suggested that one might replace the 0-1 loss $\ell(\alpha)$ by a convex surrogate $\varphi(\alpha)$ so that the minimization is tractable, where φ is differentiable, decreasing, and strictly convex (Zhang (2004); Bartlett et al. (2006); Nguyen et al. (2009)). Thus, we define $R_\varphi(\beta) = E\{\varphi(Y \beta^T X)\}$ to be the φ -risk, and look to find that the minimizer of $R_\varphi(\beta)$ as a reasonable surrogate for the minimizer of $R(\beta)$, that we can construct a rule by minimizing the sample average

$$\hat{R}_\varphi(\beta) = \frac{1}{n} \sum_{i=1}^n \varphi(Y_i \beta^T X_i). \quad (1.3)$$

This is called convex surrogate minimization (CSM). Although our primary goal is classification, the minimizer of the risk function in (1.3) will be called

the CSM estimator of $c\beta_0$, where $c > 0$ and β_0 is in (1.1).

Convexity is an increasingly important theme (Boyd and Vandenberghe (2004)). One area in which this trend has been most salient is machine learning, where computational efficiency is imperative and many of the most prominent methods make significant use of convexity; for example, support vector machines (Cristianini and Shawe-Taylor (2000); Schölkopf and Smola (2002)) and boosting (Collins et al. (2002); Lebanon and Lafferty (2002)).

In Section 2, we establish a sufficient condition on the validity of a convex surrogate φ in CSM in the sense that $R_\varphi(\beta)$ and $R(\beta)$ share the same minimizer; this leads to a CSM classification rule that converges to the optimal rule. This sufficient condition relates φ to the function g in (1.1). We show in Section 3 that, when g is known, a CSM estimator is the same as the classical maximum likelihood estimator (MLE) if the parametric likelihood is convex; otherwise the CSM estimator differs from the MLE but is computationally more efficient because of the convex optimization.

Section 4 is devoted to the case of unknown g , the single-index semi-parametric model. We show how to use an approximate convex surrogate φ that is based on a truncated quadratic loss function. The quadratic loss function, however, depends on the derivative function of g . To avoid the estimation of the derivative function of g , we apply a kernel weighting that

enables us to use an approximate convex surrogate depending on the derivative of g at 0 only. The derivative of g at 0 does not need to be estimated since $\text{sign}(\beta_0^T X) = \text{sign}(c\beta_0^T X)$ for any $c > 0$. This method produces a classification rule that converges to the optimal rule under reasonable conditions. It does not rely on the linearity condition and is computationally simpler than such dimension-reduction methods as SIR or SAVE. We obtain the asymptotic distribution of the proposed CSM estimator and the convergence rate of the CSM classification rule. Some simulation results are presented that assess the finite sample performance of the CSM estimator and other estimators under the semiparametric setting. Technical details are given in the Supplementary Material.

2. Convex Surrogates

A basic requirement for a convex surrogate φ is that the φ -risk $R_\varphi(\beta) = E\{\varphi(Y\beta^T X)\}$ has the same minimizer as the 0-1 risk $R(\beta) = E\{\ell(Y\beta^T X)\}$. If this is true for a convex φ , then the CSM based on φ and the training data can produce a classification rule that converges to the optimal rule when the training sample size $n \rightarrow \infty$. We study this issue in two steps.

2.1. Validity of a convex surrogate

For any given φ and β ,

$$E\{\varphi(Y\beta^T X)|X = x\} = g(\beta_0^T x)\varphi(\beta^T x) + \{1 - g(\beta_0^T x)\}\varphi(-\beta^T x)$$

is the conditional φ -risk, where β_0 is the true parameter value in (1.1). With $\alpha_0 = \beta_0^T x$ and $\alpha = \beta^T x$, the conditional φ -risk in the previous express can be written as

$$C(\alpha) = g(\alpha_0)\varphi(\alpha) + \{1 - g(\alpha_0)\}\varphi(-\alpha), \quad (2.4)$$

termed the generic conditional φ -risk by Bartlett et al. (2006). If a convex function φ has the property that α_0 is a unique minimizer of the generic conditional φ -risk $C(\alpha)$ defined by (2.4), then φ is called a valid convex surrogate.

Theorem 1. *For any continuous g satisfying $0 < g(\alpha) = 1 - g(-\alpha) < 1$ for $\alpha \in (-\alpha_b, \alpha_b)$ and $g(\alpha) \neq g(\alpha_0)$ for any $\alpha \neq \alpha_0$, where $g(\alpha_b) = 1$ and $g(-\alpha_b) = 0$ (α_b may be infinity), there exists a decreasing valid convex surrogate that depends on g .*

To establish this result, we construct a decreasing convex function φ of the form

$$\varphi(\alpha) = \begin{cases} \zeta(\alpha) & 0 < \alpha < \alpha_b \\ \lambda(-\alpha) & -\alpha_b < \alpha \leq 0 \end{cases} \quad (2.5)$$

where α_b is the upper bound for α , λ is an increasing, convex and differentiable function, ζ is a decreasing and differentiable function with $\zeta(0) = \lambda(0)$, and both ζ and λ are defined on $[0, \alpha_b)$. Given λ , we look to find a decreasing convex function ζ such that the solution of $C'(\alpha) = 0$ is $\alpha = \alpha_0$, where C' is the derivative of the function C in (2.4). From the definition of C in (2.4) and φ in (2.5),

$$C'(\alpha) = \begin{cases} g(\alpha_0)\zeta'(\alpha) + \{1 - g(\alpha_0)\}\lambda'(\alpha) & 0 < \alpha < \alpha_b \\ -g(\alpha_0)\lambda'(-\alpha) - \{1 - g(\alpha_0)\}\zeta'(-\alpha) & -\alpha_b < \alpha \leq 0 \end{cases}$$

If $C'(\alpha_0) = 0$, then

$$0 = \begin{cases} g(\alpha_0)\zeta'(\alpha_0) + \{1 - g(\alpha_0)\}\lambda'(\alpha_0) & 0 < \alpha_0 < \alpha_b \\ -g(\alpha_0)\lambda'(-\alpha_0) - \{1 - g(\alpha_0)\}\zeta'(-\alpha_0) & -\alpha_b < \alpha_0 \leq 0 \end{cases}$$

Since $g(\alpha) = 1 - g(-\alpha)$, as long as λ is chosen such that $\frac{g-1}{g}\lambda'$ is integrable, the relationship between ζ and λ is

$$\zeta'(\alpha) = \frac{g(\alpha) - 1}{g(\alpha)}\lambda'(\alpha) \quad \text{or} \quad \zeta(\alpha) = \int \frac{g(\alpha) - 1}{g(\alpha)}\lambda'(\alpha)d\alpha. \quad (2.6)$$

The function ζ is convex if and only if $\frac{g(\alpha)-1}{g(\alpha)}\lambda'(\alpha)$ is an increasing function.

Given g , such a function λ can be easily constructed (see Examples 1-2).

Also, since $\lambda' > 0$, ζ is a decreasing and convex function and

$$\zeta'(0) = \frac{g(0) - 1}{g(0)}\lambda'(0) = -\lambda'(0),$$

so that φ is differentiable and continuous at $\alpha = 0$.

Without loss of generality, assume $\alpha_0 > 0$. With the chosen λ and φ given by (2.6), if $0 < \alpha < \alpha_b$,

$$C'(\alpha) = \lambda'(\alpha) \left\{ g(\alpha_0) \frac{g(\alpha) - 1}{g(\alpha)} + 1 - g(\alpha_0) \right\} = \frac{\lambda'(\alpha)}{g(\alpha)} \{g(\alpha) - g(\alpha_0)\},$$

which is 0 at $\alpha = \alpha_0$. Furthermore, since $\lambda'(\alpha) > 0$ and $g(\alpha) \neq g(\alpha_0)$ for any $\alpha \neq \alpha_0$, α_0 is the unique solution to $C'(\alpha) = 0$ for $0 < \alpha < \alpha_b$. If $-\alpha_b < \alpha \leq 0$, then

$$\begin{aligned} C''(\alpha) &= -g(\alpha_0)\lambda'(-\alpha) - \{1 - g(\alpha_0)\}\zeta'(-\alpha) \\ &= -\frac{\lambda'(-\alpha)}{g(-\alpha)} [g(-\alpha) - \{1 - g(\alpha_0)\}] \\ &= -\frac{\lambda'(-\alpha)}{g(-\alpha)} [g(\alpha_0) - g(\alpha)] < 0. \end{aligned}$$

Hence, α_0 is the unique minimizer of $C(\alpha)$ and φ in (2.5)-(2.6) is valid.

To summarize, under the parametric case, we need to find an increasing, convex, and differentiable function λ such that $\frac{g-1}{g}\lambda'$ is an increasing and integrable function. A valid surrogate φ can then be obtained by (2.5)-(2.6).

For a given g , there may be many valid convex surrogates.

Example 1 (Logistic model).

Under the logistic model, $g(\alpha) = \exp(\alpha)/\{1 + \exp(\alpha)\}$, $\alpha \in (-\alpha_b, \alpha_b)$ with $\alpha_b = \infty$. We first consider $\lambda(\alpha) = \exp(\alpha)$. Then $\zeta'(\alpha) = \frac{g(\alpha)-1}{g(\alpha)}\lambda'(\alpha) =$

-1 is a constant, and

$$\varphi(\alpha) = \begin{cases} -\alpha + 1 & \alpha \geq 0 \\ \exp(-\alpha) & \alpha < 0 \end{cases}$$

is a convex function. Without loss of generality, consider $\alpha_0 > 0$ and $\alpha > 0$,

so $\alpha = \alpha_0$ is a unique solution to

$$C'(\alpha) = -\frac{\exp(\alpha_0)}{1 + \exp(\alpha_0)} + \frac{1}{1 + \exp(\alpha_0)} \exp(\alpha) = 0.$$

Next, consider $\lambda(\alpha) = \exp(\alpha/2)$. So $\zeta'(\alpha) = -\exp(-\alpha/2)/2$, and $\varphi(\alpha) = \exp(-\alpha/2)$, the exponential loss function in Zhang (2004). Then with $\lambda(\alpha) = \exp(\alpha/3)$, $\zeta'(\alpha) = -\exp(-2\alpha/3)/3$, and

$$\varphi(\alpha) = \begin{cases} \frac{1}{2} \exp\left(-\frac{2\alpha}{3}\right) + \frac{1}{2} & \alpha \geq 0 \\ \exp\left(-\frac{\alpha}{3}\right) & \alpha < 0 \end{cases}$$

Example 2 (Truncated linear model). Let

$$g(\alpha) = \begin{cases} 0 & \alpha < -\frac{1}{2b} \\ \frac{1}{2} + b\alpha & -\frac{1}{2b} \leq \alpha \leq \frac{1}{2b} \\ 1 & \alpha > \frac{1}{2b} \end{cases}$$

where b is a constant. In this case, $\alpha_b = 1/(2b)$. If $\lambda(\alpha) = (b\alpha + 1/2)^2$, then $\zeta'(\alpha) = 2b(b\alpha - 1/2)$ is increasing in α , and $\varphi(\alpha) = (1/2 - b\alpha)^2$ for

$\alpha \leq 1/(2b)$. Since $\zeta'(1/(2b)) = 0$, $\zeta(\alpha) = 0$ for all $\alpha > 1/(2b)$. Hence,

$$\varphi(\alpha) = \begin{cases} (\frac{1}{2} - b\alpha)^2 & \alpha \leq \frac{1}{2b} \\ 0 & \alpha > \frac{1}{2b} \end{cases} \quad (2.7)$$

which is truncated quadratic loss in Bartlett et al. (2006).

2.2. The risk function and its minimizers

The risk function for the classification rule $T(X) = \text{sign}(\beta^T X)$ under the 0-1 loss is

$$\begin{aligned} R(\beta) &= E\{\ell(Y\beta^T X)\} = E[E\{\ell(Y\beta^T X)|X\}] \\ &= E [P(Y = 1, \beta^T X \leq 0|X) + P(Y = -1, \beta^T X \geq 0|X)] \\ &= \int_{\beta^T x \leq 0} g(\beta_0^T x) dF(x) + \int_{\beta^T x > 0} \{1 - g(\beta_0^T x)\} dF(x) \\ &= \int_{\beta^T x \leq 0} \{2g(\beta_0^T x) - 1\} dF(x) + \int \{1 - g(\beta_0^T x)\} dF(x), \end{aligned} \quad (2.8)$$

where F is the joint cumulative distribution function of X . Figure 1 shows a 3d plot of the function $R(\beta)$ for $g(\beta^T X) = \exp(\beta_1 x_1 + \beta_2 x_2) / \{1 + \exp(\beta_1 x_1 + \beta_2 x_2)\}$, and (x_1, x_2) is bivariate normal with mean zero and identity matrix as the covariance matrix. From Figure 1, when $\beta_1 = \beta_2$, the risk function $R(\beta)$ is minimized.

In general, it can be seen from (2.8) that if we choose $\beta = c\beta_0$ with a constant $c > 0$, then the first integral on the right side of (2.8) is 0 and

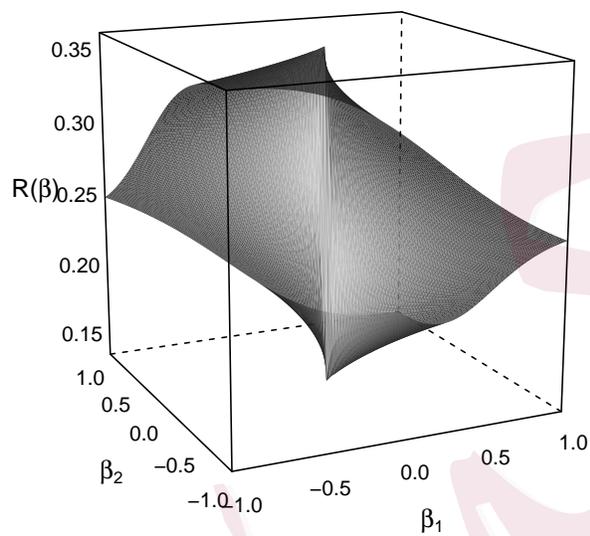


Figure 1: The plot of 0-1 risk $R(\beta)$

$R(\beta)$ reaches its minimum $\int \{1 - g(\beta_0^T x)\} dF(x)$, $c\beta_0$ is a minimizer of $R(\beta)$ for any $c > 0$ (the minimizer is not unique). The proof of the following is given in the Supplementary Material.

Lemma 1. *If the non-constant part of X has a density f , and f and g are continuous, then $R(\beta)$ is differentiable at $\beta = c\beta_0$ for any constant $c > 0$ and $\partial R(\beta)/\partial \beta|_{\beta=c\beta_0} = 0$.*

We now turn to the φ -risk for convex surrogate φ , $R_\varphi(\beta) = E\{\varphi(Y\beta^T X)\}$.

We take $\Psi(\beta_0)$ to be a set of valid convex surrogates φ ,

$$\Psi(\beta_0) = \{\varphi : \text{convex, differentiable, for any } x \quad (2.9)$$

$$g(\beta_0^T x)\varphi'(\beta_0^T x) + \{1 - g(\beta_0^T x)\}\varphi'(-\beta_0^T x) = 0\}.$$

From Theorem 1, $\Psi(\beta_0)$ is not empty. Unlike the 0-1 risk, for any $\varphi \in \Psi(\beta_0)$, the minimizer of φ -risk is unique. The proof of the following is in the Supplementary Material.

Lemma 2. *Let $\varphi \in \Psi(\beta_0)$ with finite $\int \sup_{\beta \in \mathcal{N}} |\varphi'(\beta^T x)| x dF(x)$ and $\int \sup_{\beta \in \mathcal{N}} |\varphi''(\beta^T x)| x^T x dF(x)$, where \mathcal{N} is a neighborhood of β_0 . Then, the unique minimizer of $R_\varphi(\beta)$ over β is at $\beta = \beta_0$.*

By Lemma 1, the minimizers of the 0-1 risk $R(\beta)$ form a set $\{c\beta_0 : c > 0\}$, and, by Lemma 2, the minimizer of $R_\varphi(\beta)$ is unique for each $\varphi \in \Psi$ under minor conditions. For any positive constant c , $c\beta_0$ is actually a minimizer of the φ_c -risk with $\varphi_c(\alpha) = \varphi(c\alpha)$, which is a valid convex surrogate if φ is a valid convex surrogate.

These conclusions help us to simplify the problem in the semiparametric case by ignoring an unknown constant (slope).

3. Applications in Parametric Models

When g is known, model (1.1) is parametric and we can apply maximum-likelihood estimation (MLE) to estimate the unknown β_0 . The likelihood based on training data (Y_i, X_i) , $i = 1, \dots, n$, is

$$L(\beta) = \prod_{i=1}^n g(\beta^T X_i)^{\frac{1+Y_i}{2}} \{1 - g(\beta^T X_i)\}^{\frac{1-Y_i}{2}},$$

the joint probability mass function of Y_1, \dots, Y_n conditioned on X_i , $i = 1, \dots, n$. Classical asymptotic theory shows that the MLE is asymptotically normal with mean β_0 and asymptotic covariance matrix

$$\frac{1}{n} \left[E \left\{ X X^T \frac{g'^2(\beta_0^T X)}{g(\beta_0^T X)g(-\beta_0^T X)} \right\} \right]^{-1} \quad (3.10)$$

under the conditions on g in Theorem 1, where g' is the derivative of g , and that the MLE is optimal in the sense that any other asymptotically normal estimator of β_0 has asymptotic covariance matrix no smaller than that in (3.10) in terms of matrix ordering.

The CSM estimator based on a convex surrogate φ is obtained by minimizing the empirical φ -risk defined in (1.3),

$$\frac{1}{n} \sum_{i=1}^n \varphi(Y_i \beta^T X_i).$$

Let φ be given by (2.5) with $\zeta'(\alpha) = \frac{g(\alpha)-1}{g(\alpha)}\lambda'(\alpha)$. Then

$$\varphi(Y_i\beta^T X_i) = \begin{cases} \frac{1+Y_i}{2}\zeta(\beta^T X_i) + \frac{1-Y_i}{2}\lambda(\beta^T X_i) & \text{if } \beta^T X_i > 0 \\ \frac{1+Y_i}{2}\lambda(-\beta^T X_i) + \frac{1-Y_i}{2}\zeta(-\beta^T X_i) & \text{if } \beta^T X_i \leq 0, \end{cases}$$

$$\frac{\partial\varphi(Y_i\beta^T X_i)}{\partial\beta} = \begin{cases} \frac{1+Y_i}{2}X_i\frac{g(\beta^T X_i)-1}{g(\beta^T X_i)}\lambda'(\beta^T X_i) + \frac{1-Y_i}{2}X_i\lambda'(\beta^T X_i) & \text{if } \beta^T X_i > 0 \\ -\frac{1+Y_i}{2}X_i\lambda'(-\beta^T X_i) - \frac{1-Y_i}{2}X_i\frac{g(-\beta^T X_i)-1}{g(-\beta^T X_i)}\lambda'(-\beta^T X_i) & \text{if } \beta^T X_i \leq 0 \end{cases}$$

$$= \frac{X_i\lambda'(|\beta^T X_i|)}{2g(|\beta^T X_i|)} [2g(\beta^T X_i) - 1 - Y_i].$$

Consequently, the CSM estimator is obtained by solving

$$H(\beta) = \frac{\partial}{\partial\beta} \left\{ \sum_{i=1}^n \varphi(Y_i\beta^T X_i) \right\} = \sum_{i=1}^n \frac{X_i\lambda'(|\beta^T X_i|)}{2g(|\beta^T X_i|)} [2g(\beta^T X_i) - 1 - Y_i] = 0.$$

Since $H(\beta)$ is a sum of independent and identically distributed random vectors, the solution is asymptotically normal with mean β_0 and asymptotic covariance matrix

$$n^{-1}[E\{H'(\beta_0)\}]^{-1}\text{Cov}\{H(\beta_0)\}[E\{H'(\beta_0)\}]^{-1}, \quad (3.11)$$

where $H'(\beta) = \partial H(\beta)/\partial\beta$,

$$E\{H'(\beta_0)\} = E \left\{ XX^T \frac{\lambda'(|\beta_0^T X|)g'(\beta_0^T X)}{g(|\beta_0^T X|)} \right\},$$

$$\text{Cov}\{H(\beta_0)\} = E \left\{ XX^T \frac{\lambda'^2(|\beta_0^T X|)g(\beta_0^T X)g(-\beta_0^T X)}{g^2(|\beta_0^T X|)} \right\}.$$

Comparing (3.10) and (3.11), we conclude that the matrices in (3.10) and (3.11) are the same if and only if the λ function satisfies $\lambda'(\alpha) = \frac{g'(\alpha)}{1-g(\alpha)}$, or $\varphi(\alpha) = -\log\{g(\alpha)\}$ provided $-\log\{g(\alpha)\}$ is convex.

Conclusion 1. Thus, when $-\log\{g\}$ is a convex function and g satisfies the conditions in Theorem 1, the CSM with $\varphi = -\log\{g\}$ is equivalent to the MLE. The CSM estimators with other φ 's have asymptotic covariance matrices given by (3.11) and are asymptotically less efficient than the MLE, but may be computationally more efficient.

Example 1 (continued). Consider the logistic model with $g(\alpha) = \exp(\alpha)/\{1 + \exp(\alpha)\}$. If model (1.1) is viewed as a generalized linear model, then the logistic model corresponds to the canonical link (McCullagh and Nelder (1989)). It is well known that $-\log$ of likelihood is convex in this case. In fact, $-\log\{g(\alpha)\} = \log\{1 + \exp(-\alpha)\}$ is convex. The CSM with $\varphi(\alpha) = \log\{1 + \exp(-\alpha)\}$ is the same as the MLE.

Consider the CSM with the convex surrogate $\varphi(\alpha) = \exp(-\alpha/2)$ given in Example 1 in Section 2. From the previous discussion, this CSM is not equivalent to the MLE. We compared in a simulation the MLE and CSM with $\varphi(\alpha) = \exp(-\alpha/2)$ in a logistic model with a 5-dimensional $\beta_0 = (\beta_{01}, \dots, \beta_{05})^T$ and $X = (1, \xi_2, \dots, \xi_5)^T$, where ξ_2, \dots, ξ_5 are independent standard normal random variables. The sample size was $n = 200$ and the

Table 1: Simulation mean, rmse, and time under the logistic model

		simulation size = 1,000	
		$n = 200$	
true ratio		CSM	MLE
$\beta_{02}/\beta_{01} = 0.5$	mean	0.524	0.521
	rmse	0.210	0.204
$\beta_{03}/\beta_{01} = 1$	mean	1.036	1.030
	rmse	0.256	0.248
$\beta_{04}/\beta_{01} = 0.5$	mean	0.529	0.526
	rmse	0.213	0.211
$\beta_{05}/\beta_{01} = 0$	mean	0.001	0.003
	rmse	0.196	0.188
	time in seconds	49.87	274.28

simulation size was 1,000. Table 1 shows the means and root mean squared errors (rmse) of the estimated ratios β_{0j}/β_{01} , $j = 2, \dots, 5$. The true values of the ratios and the time used to compute the estimators are also included in the table. All estimators were computed using the R function “optimize”.

From Table 1, both estimators are almost unbiased and the CSM es-

imator has a larger but comparable rmse. However, the CSM is much faster.

Example 1A (probit model). Consider probit model, $g(\alpha)$ in (1.1) is $\Phi(\alpha)$, the standard normal cumulative distribution function. We can show that $\varphi(\alpha) = -\log \Phi(\alpha)$ is convex so that the conclusions are the same as those in the logistic model. We have

$$\varphi'(\alpha) = -\frac{\Phi'(\alpha)}{\Phi(\alpha)} \quad \text{and} \quad \varphi''(\alpha) = -\frac{\Phi''(\alpha)\Phi(\alpha) - \{\Phi'(\alpha)\}^2}{\{\Phi(\alpha)\}^2}.$$

For the normal, $\Phi''(\alpha) = -\alpha\Phi'(\alpha)$, so

$$\varphi''(\alpha) = \frac{\Phi'(\alpha)}{\{\Phi(\alpha)\}^2} \{\alpha\Phi(\alpha) + \Phi'(\alpha)\} = \frac{\Phi'(\alpha)}{\{\Phi(\alpha)\}^2} \int_{-\infty}^{\alpha} \Phi(t) dt > 0,$$

which proves that $\varphi(\alpha) = -\log \Phi(\alpha)$ is convex.

Example 2 (continued). Consider the truncated linear model

$$P(Y = 1|X) = \begin{cases} 0 & \beta_0^T X \leq -\frac{1}{2} \\ \frac{1}{2} + \beta_0^T X & -\frac{1}{2} < \beta_0^T X \leq \frac{1}{2} \\ 1 & \beta_0^T X > \frac{1}{2} \end{cases}$$

with $\beta_0 = (\beta_{01}, \dots, \beta_{05})^T = (0.25, 0.5, 0.25, 0.5, 0.5)^T$ and X the same as that in Example 1. Here $-\log$ of likelihood is not convex. If we use the truncated quadratic loss in (2.7) (Bartlett et al. (2006)) as the convex surrogate, the CSM and MLE differ. The simulation results given in Table 2 show that the

MLE is worse than the CSM when $n = 200$ in terms of rmse; although the MLE is asymptotically optimal, when $-\log\{g(\alpha)\}$ is not convex, the MLE requires a large n to appreciate the asymptotic effect. To show this we ran an additional simulation with $n = 500$. The results are in Table 2 and show that the MLE is slightly better than the CSM. The computational gain in using the CSM is larger in this case because the MLE is not a convex optimization.

We conclude that when $-\log\{g(\alpha)\}$ is not convex, the CSM can be used as a substitute for the MLE for computational saving. Because of the complexity in computing the MLE, the CSM estimators may be better than the MLE with not very large n , although they are asymptotically less efficient than the MLE.

When $-\log\{g(\alpha)\}$ is not convex, there may not exist an optimal CSM estimator in terms of either estimation efficiency or computation complexity. Because the CSM is mainly for computational saving, it is not necessary to find a φ having the optimal computation efficiency. Using the asymptotic covariance matrix given by (3.11), we can perform some numerical studies to choose a surrogate φ having reasonable estimation efficiency. For example, in the three examples in this section, we have found some good surrogates.

Table 2: Simulation mean, rmse, and time under the truncated linear model

		simulation size = 1,000			
		$n = 200$		$n = 500$	
true ratio		CSM	MLE	CSM	MLE
$\beta_{02}/\beta_{01} = 2$	mean	2.075	2.095	2.025	2.018
	rmse	0.489	0.588	0.257	0.243
$\beta_{03}/\beta_{01} = 1$	mean	1.044	1.060	1.008	1.006
	rmse	0.305	0.355	0.159	0.142
$\beta_{04}/\beta_{01} = 2$	mean	2.086	2.110	2.022	2.016
	rmse	0.504	0.609	0.258	0.251
$\beta_{05}/\beta_{01} = 2$	mean	2.083	2.108	2.022	2.012
	rmse	0.510	0.613	0.259	0.251
	time in seconds	53.22	387.55	101.56	829.39

4. Applications in Semiparametric Models

We now consider model (1.1) with unknown g and β_0 , a semiparametric model. Although Theorem 1 shows the existence of a valid convex surrogate, when g is unknown it is difficult to find a valid convex surrogate. We propose a method of constructing an approximate convex surrogate and establish its

asymptotic properties in Section 4.1, then provide some empirical results in Section 4.2.

4.1. Method and theory

Our idea is to first linearize g at 0 and consider the truncated quadratic loss in (2.7), which produces a valid convex surrogate φ when g is actually linear. After obtaining a φ , we apply kernel weighting to overcome the difficulty that g is not linear.

Consider the Taylor expansion of $g(\alpha)$ at $\alpha = 0$,

$$g(\alpha) \approx g(0) + g'(0)\alpha. \quad (4.12)$$

Although $g(0) = 1/2$, the derivative $g'(0)$ is unknown. From the discussion at the end of Section 2.2, if $\varphi(\alpha)$ is valid, so is $\varphi(c\alpha)$ for any $c > 0$. Thus, we need not estimate the unknown $g'(0)$. If g is actually linear, then \approx in (4.12) is an equality, and, based on Example 2, we can use the convex surrogate

$$\tilde{\varphi}(\alpha) = \begin{cases} (\frac{1}{2} - \alpha)^2 & \alpha \leq \frac{1}{2} \\ 0 & \alpha > \frac{1}{2} \end{cases} \quad (4.13)$$

Still, (4.12) is an approximation that only holds for α near 0 when g is not linear. Therefore, minimizing the $\tilde{\varphi}$ -risk $\hat{R}_{\tilde{\varphi}}(\beta) = n^{-1} \sum_{i=1}^n \tilde{\varphi}(Y_i \beta^T X_i)$ may not lead to a satisfactory result since $Y_i \beta^T X_i$ may not be close to 0 for all i .

To overcome this, we apply kernel weighting in conjuncture with the convex surrogate $\tilde{\varphi}$ in (4.13). Minimizing $\sum_{i=1}^n \tilde{\varphi}(Y_i \beta^T X_i)$ is the same as solving

$$\frac{1}{n} \sum_{i=1}^n \tilde{\varphi}'(Y_i \beta^T X_i) Y_i X_i = 0. \quad (4.14)$$

Let K be a symmetric probability density function, a kernel with support $[-1, 1]$ and

$$B_K = \int_{-1}^1 u^2 K(u) du < \infty \quad \text{and} \quad V_K = \int_{-1}^1 K^2(u) du < \infty,$$

and let $h > 0$ be a bandwidth and $K_h(t) = K(t/h)/h$. Then, we replace (4.14) by the kernel weighted version,

$$\frac{1}{n} \sum_{i=1}^n \tilde{\varphi}'(Y_i \beta^T X_i) Y_i X_i K_h(\beta^T X_i) = 0. \quad (4.15)$$

By suitably choosing the bandwidth h , the solution of (4.15) is asymptotically valid.

Solving (4.15) is not a convex optimization since the weight $K_h(\beta^T X_i)$ involves β . We have to apply an algorithm such as Newton's method. This is the price we pay for using a semiparametric model.

The solution to (4.15) estimates $g'(0)\beta_0$, $g'(0) > 0$. The proof of the following is given in the Supplementary Material.

Theorem 2. *Let $\hat{\beta}$ the solution of (4.15). Assume the parameter space for β^0 is a compact set; model (1.1) holds with an unknown g that is third*

order differentiable with bounded third order derivative; K satisfies the basic kernel conditions, $h \rightarrow 0$, $nh \rightarrow \infty$, and $nh^5 \rightarrow 0$ as $n \rightarrow \infty$; and the non-constant part of X has a continuous density $f > 0$. Assume further that the matrix

$$D = \frac{1}{|\beta_{0p}|g'(0)} \int \begin{pmatrix} 1 & z^T \\ z & zz^T \end{pmatrix} f(z) dx_2 \cdots dx_{p-1} \quad (4.16)$$

is positive definite, where z is the $(p-1)$ -dimensional vector whose first $p-2$ components are x_2, \dots, x_{p-1} and the last component is $-(\beta_{01} + \beta_{02}x_2 + \cdots + \beta_{0(p-1)}x_{p-1})/\beta_{0p}$, and β_{0j} is the j th component of β_0 . Then, as $n \rightarrow \infty$,

- (i) $\hat{\beta}$ converges in probability to $g'(0)\beta_0$;
- (ii) $(nh)^{1/2}\{\hat{\beta} - g'(0)\beta_0\}$ converges in distribution to the p -dimensional multivariate normal distribution with mean 0 and covariance matrix $V_K D^{-1}/4$;
- (iii) based on the asymptotic mean squared error of $\hat{\beta} - g'(0)\beta_0$, the optimal choice of h is $h \asymp n^{-1/5}$, where $a \asymp b$ means $a = O(b)$ and $b = O(a)$;
- (iv) If $R(\beta)$ is the 0-1 risk defined at (1.2), and if the density f is continuously differentiable, then, $R(\hat{\beta}) = R(\beta_0) + O_p(n^{-4/5})$ when $h \asymp n^{-1/5}$.

In applications we need to choose a bandwidth h for a fixed sample size n . There is a rich literature on bandwidth selection in applying a kernel method. One can apply cross-validation, leaving out one data point at a

time, and choosing the value of h that minimizes

$$\text{CV}(h) = \frac{1}{n} \sum_{i=1}^n \ell(Y_i \hat{\beta}_{(-i)}^T X_i),$$

where $\hat{\beta}_{(-i)}$ is the solution to (4.15) with the i th term in the summation deleted. Here $\ell(Y_i \hat{\beta}_{(-i)}^T X_i)$ is the loss when we classify the i th subject in the training data set by using the CSM classification rule based on the data set with (Y_i, X_i) removed from the original data set. Thus, $\text{CV}(h)$ quantifies the classification accuracy of the CSM based on h .

4.2. Simulation results

This section presents some results from two simulation studies under the semiparametric model (1.1) with unknown g and β_0 , so as to illustrate the finite sample performance of the CSM and compare it with the estimation-based methods SIR, SAVE, DR, EPFC, and LAD. These five are dimension-reduction methods, which can be applied by using the available LDR package in Matlab.

In the first simulation study we generated X_1, \dots, X_n from a multivariate normal distribution so that the linearity condition described in Section 1 was satisfied and all estimators were asymptotically normal with mean $c\beta_0$ for some $c > 0$. In the second simulation study X_1, \dots, X_n were generated from a distribution that did not satisfy the linearity condition. In both cases

all components of X were non-constant, and we knew that the intercept was 0.

4.2.1. Results under a multivariate normal X

In the first simulation study, $P(Y = 1|X) = \exp(\beta_0^T X)/[1 + \exp(\beta_0^T X)]$ and $X \sim N_5(0, I_5)$, where $\beta_0 = (2, 1, 2, 1, 0)^T$ is 5-dimensional and I_5 is the identity matrix of order 5. From the previous discussion we know that it is enough to estimate $c\beta_0$ for classification. Thus, we considered the estimation of the ratios β_{0j}/β_{01} , $j = 2, \dots, 5$ with the true value $(0.5, 1, 0.5, 0)$, where β_{0j} is the j th component of β_0 .

The results in Table 3 are based on $n = 100$ and the simulation size 1,000. We calculated the means and root mean squared errors (rmse) of estimators of β_{0j}/β_{01} based on the SIR, SAVE, DR, EPFC, LAD, and C-SM. To evaluate the performance of the classification, in each simulation run we generated another sample $\{(\tilde{Y}_1, \tilde{X}_1), \dots, (\tilde{Y}_m, \tilde{X}_m)\}$ of size $m = 50$ from the distribution of (Y, X) , independent of $\{(Y_1, X_1), \dots, (Y_n, X_n)\}$, and calculated the sample average of the loss, $\hat{R}(\hat{\beta}) = m^{-1} \sum_{i=1}^m \ell(\tilde{Y}_i \hat{\beta}^T \tilde{X}_i)$, for $\hat{\beta}$ obtained using each method under consideration; this can be treated as an estimate of the misclassification rate by using $\hat{\beta}$. The simulation mean and rmse of $\hat{R}(\hat{\beta})$ for each method is included in Table 3.

From this table, all the methods have good performances, except that

Table 3: Simulation results for the first simulation study

simulation size = 1,000

		$n = 100$					
true value		SIR	SAVE	DR	EPFC	LAD	CSM
$\beta_{02}/\beta_{01} = 0.5$	mean	0.512	0.544	0.516	0.510	0.511	0.509
	rmse	0.199	0.408	0.221	0.208	0.202	0.198
$\beta_{03}/\beta_{01} = 1$	mean	1.028	1.003	1.027	1.030	1.024	1.030
	rmse	0.283	0.976	0.301	0.298	0.280	0.278
$\beta_{04}/\beta_{01} = 0.5$	mean	0.516	0.493	0.515	0.518	0.519	0.517
	rmse	0.213	0.702	0.218	0.220	0.217	0.202
$\beta_{05}/\beta_{01} = 0$	mean	0.002	-0.044	-0.000	0.002	0.001	0.003
	rmse	0.171	0.687	0.192	0.181	0.178	0.162
$R(\beta_0) = 0.157$	mean	0.168	0.182	0.169	0.169	0.168	0.168
	rmse	0.052	0.069	0.052	0.052	0.052	0.051

SAVE has a larger rmse and slightly worse misspecification rate than the other methods.

4.2.2. Results under an asymmetric X

In the second simulation study, $P(Y = 1|X) = \Phi(\beta_0^T X)$ and each com-

ponent of X had an asymmetric mixture distribution $\frac{1}{2}N(1, 2) + \frac{1}{2}N(-\frac{1}{2}, 1)$. The vector β_0 was 6-dimensional with the true ratios $(0.5, 1, 0.5, 0, 0)$. The simulation results are given in Table 4.

Under this setting, the linearity condition described in Section 1 does not hold and the asymptotic behaviors of SIR, SAVE, DR, EPFC, and LAD are unknown. Theorem 2 for the CSM does not require the linearity condition and, from Table 4, it is better than the other five methods in terms of rmse. SAVE has a substantially larger rmse than all other methods, and also has the worst misspecification rate. The CSM has the best misspecification rate although the SIR, DR, EPFC, and LAD have misspecification rates close to that of the CSM.

Supplementary Materials

The supplementary material contains proofs of Lemmas 1-2 and Theorem 2.

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Table 4: Simulation results for the second simulation study

simulation size = 1,000

		$n = 100$					
true value		SIR	SAVE	DR	EPFC	LAD	CSM
$\beta_{02}/\beta_{01} = 0.5$	mean	0.545	0.488	0.544	0.547	0.523	0.524
	rmse	0.181	0.800	0.185	0.186	0.169	0.141
$\beta_{02}/\beta_{01} = 1$	mean	1.022	1.056	1.028	1.020	1.025	1.020
	rmse	0.204	1.455	0.212	0.214	0.205	0.172
$\beta_{02}/\beta_{01} = 0.5$	mean	0.540	0.454	0.536	0.541	0.513	0.516
	rmse	0.172	1.297	0.173	0.177	0.164	0.139
$\beta_{02}/\beta_{01} = 0$	mean	0.007	0.001	0.004	0.009	0.006	0.020
	rmse	0.139	0.337	0.152	0.144	0.128	0.111
$\beta_{02}/\beta_{01} = 0$	mean	-0.004	-0.020	-0.008	-0.005	0.002	0.017
	rmse	0.141	0.563	0.156	0.144	0.129	0.112
$R(\beta_0) = 0.064$	mean	0.083	0.104	0.085	0.085	0.082	0.076
	rmse	0.043	0.079	0.043	0.043	0.041	0.039

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School of Statistics, East China Normal University, Shanghai 200241, China.

E-mail: cxiong531@163.com

Department of Statistics, University of Wisconsin-Madison, Madison, WI 53706, U.S.A.

E-mail: shao@stat.wisc.edu

REFERENCES₃₂

LPMC and Institute of Statistics, Nankai University, Tianjin 300071, China.

E-mail: leiwang.stat@gmail.com

Statistica Sinica