Consistent Cross-Validation for Tuning Parameter Selection in High-Dimensional Variable Selection

Yang Feng∗ and Yi Yu†

Abstract

Asymptotic behavior of the tuning parameter selection in the standard cross-validation methods is investigated for the high-dimensional variable selection problem. It is shown that the shrinkage problem with the Lasso penalty is not always the true reason for the over-selection phenomenon in the cross-validation based tuning parameter selection. After identifying the potential problems with the standard cross-validation methods, we propose a new procedure, Consistent Cross-Validation (CCV), for selecting the optimal tuning parameter. CCV is shown to enjoy the tuning parameter selection consistency under certain technical conditions. Extensive simulations and real data analysis support the theoretical results and demonstrate that CCV also works well in terms of prediction.

1 Introduction

In recent years, massive high-throughput and high-dimensional datasets are generated as a result of technological advancement in many fields. Such data are featured by the large number of variables $p$ as compared with the sample size $n$. Usually, it is assumed that there are only a few important variables that contribute to the response. Variable selection is a natural tool to discover the important variables. We refer to Fan and Lv (2010) for an overview of variable selection in high-dimensional feature space.

The first attempt to variable selection was the $\ell_0$ type regularization methods, including AIC (Akaike, 1973), $C_p$ (Mallows, 1973) and BIC (Schwarz, 1978), which work well in low dimensional cases, but computationally prohibitive in high-dimensional settings. As a result, numerous efforts have been made to modify the $\ell_0$ type regularization to reduce the computational burden. Among them, Tibshirani (1996) proposed Lasso, which is the $\ell_1$ penalty, or equivalently, Chen and Donoho (1994) proposed Basis Pursuit. Also, folded-concave penalties such as SCAD (Fan and Li, 2001) and MCP (Zhang, 2010) have been proposed and widely used over the years. All of these variable selection procedures were shown to have good theoretical results. For Lasso, prediction and selection performances were studied in Greenshtein and Ritov (2004).

∗Department of Statistics, Columbia University, New York, NY, USA. yangfeng@stat.columbia.edu
†Statistical Laboratory, University of Cambridge, UK. y.yu@statslab.cam.ac.uk
Meinshausen and Bühlmann (2006), Zhao and Yu (2006), Bunea et al. (2007), Zhang and Huang (2008), Meinshausen and Yu (2009), Bickel et al. (2009), Zhang (2010), among others. For folded-concave penalties, such as SCAD and MCP, their theoretical properties were studied in Fan and Li (2001), Fan and Lv (2011), Zhang (2010) and Feng et al. (2013).

It is desirable to develop efficient algorithms for calculating the solution path of the coefficient vector as the tuning parameter varies. For Lasso, least angle regression (LARS) (Efron et al., 2004), or homotopy (Osborne et al., 2000) is an efficient method for computing the entire path of Lasso solutions in the linear regression case. For folded-concave penalties including SCAD and MCP, Fan and Li (2001) used the Local Quadratic Approximation (LQA); Zou and Li (2008) proposed the Local Linear Approximation (LLA), which makes a local linear approximation to the penalty, thereby yielding an objective function that can be optimized by using the LARS algorithm; Zhang (2010) proposed the penalized linear unbiased selection algorithm (PLUS), which is designed for linear regression penalized by quadratic spline penalties, including Lasso, SCAD and MCP. Recently, coordinate descent methods have received a majority of attention in high-dimensional setting, including Fu (1998), Shevade and Keerthi (2003), Krishnapuram et al. (2005), Genkin et al. (2007), Friedman et al. (2007), Wu and Lange (2008), among others. Other work on penalized linear regression includes Hastie et al. (2004), Daubechies et al. (2004), Kim et al. (2007), She (2012), Yu and Feng (2013a), among others.

In all the existing algorithms for calculating the solution path for penalized estimators, there is a tuning parameter which controls the penalty level. As it turns out, selecting the optimal tuning parameter is both important and difficult. There has been an abundance of research on using certain kinds of information criteria to select the tuning parameter. Tibshirani (1996) used generalized cross-validation (GCV) style statistics, Efron et al. (2004) used $C_p$ style statistics. Zou et al. (2007) derived a consistent estimator of degrees of freedom of the Lasso in the $C_p$, AIC, and BIC criteria. But from simulation experience, all these traditional methods when applied to the Lasso, tend to over select. Chen and Chen (2008) proposed extended-BIC, by adding an extra term with respect to $p$ into the criterion function. Zhang et al. (2010) proposed the generalized information criterion (GIC), which makes a connection between the classical variable selection criteria and the regularization parameter selection for the nonconcave penalized likelihood approaches. Recently, Fan and Tang (2012) studied the GIC for a diverging $p$ scenario. Other related work includes selection of the tuning parameter through joint estimation of $\beta$ and $\sigma$ (Städler et al., 2010; Sun and Zhang, 2011).

Besides the many information-type criteria, another popular method for selecting the tuning parameter is cross-validation, which is a data-driven method. A vast theoretical work has been done for cross-validation in the classic linear regression models. For example, leave-one-out cross-validation (CV(1)) is shown to be asymptotically equivalent to AIC, the $C_p$, the jackknife, and the bootstrap (Stone, 1977; Efron, 1983, 1986). Shao (1993) gave rigorous proof of the inconsistency of CV(1) for the classical linear regression model, meanwhile he gave the proper size of construction and validation sets in leave-$n_v$-out cross-validation (CV($n_v$)), under which cross-validation achieves the model selection consistency. Here, by construction and validation datasets
we mean the subsets of the complete dataset used to construct and validate the estimators in cross-validation splits. Zhang (1993) studied multifold cross-validation and r-fold cross-validation in classic linear regression models. Yu and Feng (2013b) gave some modifications to the cross-validation for penalized least squares estimators, which have good numerical performance but lack theoretical support.

To calculate the solution path for high-dimensional variable selection methods, there are several packages available in R, including lars (Efron et al., 2004), glmnet (Friedman et al., 2007), glmpath (Park and Hastie, 2007), plus (Zhang, 2010), ncvreg (Breheny and Huang, 2011), apple (Yu and Feng, 2013a), among others. In all these packages, the default tuning parameter selection method is K-fold cross-validation. Nevertheless, researchers have realized that the K-fold cross-validation in high-dimensional settings tends to be too conservative in the sense that it will select plenty of noise variables. As mentioned in Zhang and Huang (2008), the theoretical justification of cross-validation based tuning parameter is unclear for model-selection purposes.

Another related work is the relaxed Lasso (Meinshausen, 2007) with LARS-OLS (Efron et al., 2004) as its special case. The relaxed Lasso is a two-stage method, with the penalty relaxed at the second stage, only operating on those variables being selected at the first stage. In Section 3.4 of Meinshausen (2007), the author conjectured that the K-fold cross-validation will achieve model selection consistency. Different from Meinshausen (2007), in this paper we mainly focus on tuning parameter selection instead of proposing a variant of Lasso procedure, and give the rigorous discussion on the asymptotic behavior of cross-validation.

The contribution of the paper is two-fold: (1) a thorough investigation is conducted for the advantages and drawbacks of the commonly used cross-validation methods for tuning parameter selection in the penalized estimation methods, and (2) a new cross-validation method is proposed, which is shown to be consistent for a wide range of penalty functions under the generalized linear model framework.

The rest of the paper is organized as follows. In Section 2, the model setup is introduced, with notations and technical conditions explained. In Section 3, we study the asymptotic behavior of the cross-validation methods under high-dimensional settings, and point out the potential drawbacks. A new tuning parameter selection method Consistent Cross-Validation (CCV) is proposed in Section 4. Simulations and real data analysis results are presented in Sections 5 and 6, respectively. We conclude with a short discussion in Section 7. The majority of the technical details are relegated to the Appendix.

2 Model Setup and Conditions

2.1 Penalized Likelihood Estimators for GLM

Suppose we have n iid observation pairs \((x_i, y_i), i = 1, \ldots, n\), where \(x_i\) is a p-dimensional predictor and \(y_i\) is the response. We assume the conditional distribution of \(y\) given \(x\) belongs to an exponential family with the canonical link; that is, it has the following density function,

\[
f(y; x, \beta) = c(y, \phi) \exp\left(\frac{(y \theta - b(\theta))}{a(\phi)}\right),
\]
where $\theta = x^T \beta$ and $\phi \in (0, \infty)$ is the dispersion parameter. Here, $\beta$ is the parameter of interest, and it also represents the true parameter, with $\|\beta\|_0 = d_0 < n$, where for a vector $a$, $\|a\|_0 = \#\{j : a_j \neq 0\}$. In the following, unless otherwise stated, denote by $\|\cdot\|$ as the $\ell_2$ norm of vector or matrix, depending on the specific situation. Let $O = \{j : \beta_j \neq 0\}$ be the true model. Then up to an affine transformation, the log-likelihood of the sample is given by

$$\ell(y; \beta) = n^{-1} \sum_{i=1}^{n} [y_i \theta_i - b(\theta_i)].$$

One popular variable selection scheme is to minimize a penalized negative log-likelihood function, i.e.,

$$\hat{\beta} = \arg\min_{\beta} [-\ell(y; \beta) + p_\lambda(\beta)],$$

(1)

where $p_\lambda(\cdot)$ is the penalty function.

In this paper, we only consider separable penalties; that is, there exists a non-negative function $\rho(\cdot)$, such that for any vector $\beta = (\beta_1, \cdots, \beta_p)$, the penalty function $p_\lambda(\cdot)$ satisfies

$$p_\lambda(\beta) = \sum_{j=1}^{p} \rho(|\beta_j|; \lambda, \gamma),$$

(2)

where $\lambda$ and $\gamma$ are the parameters of the penalty function. Both convex and folded-concave penalties are in the scope of this paper. For convex penalty, such as Lasso (Tibshirani, 1996), $\gamma = \infty$; while for folded-concave penalty, such as SCAD (Fan and Li, 2001) and MCP (Zhang, 2010), $0 < \gamma < \infty$. In the penalty function (2), $\gamma$ is usually a predetermined parameter controlling the concavity of the penalty, and we will only focus on studying the solution path as $\lambda$ changes in this paper.

### 2.2 Cross-Validation for Path Algorithm

In the following, we provide an outline of the state-of-the-art algorithm on using cross-validation for tuning parameter selection for (1). To get the idea across, we use the general leave-$n_v$-out cross-validation $CV(n_v)$, which includes the popular $K$-fold cross-validation and leave-one-out cross-validation as special cases.

**Algorithm 1. (Cross-Validation for Path Algorithm)**

1. **S1.** Compute the solution path with the whole dataset. A sequence of solutions $\hat{\beta}(\lambda)$ is generated as a function of the penalty level $\lambda$.

2. **S2.** Randomly split the whole dataset into $\{(x_i, y_i), i \in s\}$ (the validation set) and $\{(x_i, y_i), i \in s^c\}$ (the construction set) $r$ times, where $s$ is a subset of $\{1, \cdots, n\}$ containing $n_v$ integers and $s^c$ is its complement containing $n_c$ integers. For each split $j = 1, \cdots, r$, compute the solution path $\hat{\beta}^{(j)}(\lambda)$ for the construction data in $s^c$. Then, compute the loss function (e.g., negative log-likelihood) on the validation data in $s$ with $\hat{\beta}^{(j)}(\lambda)$. 

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Suppose the loss function employed in S2 is the negative log-likelihood; that is, for each solution path, respectively. Averaging is performed over the same tuning parameter or the same position on the scenarios, using the sequence in S1 or their own adaptive sequences. And in S3, the tuning parameter sequences for sub-samples also have two respective R packages (e.g., glmnet, ncvreg, apple) generate a decreasing equal-spaced log-scale tuning parameter sequence, with the largest one forcing the estimator equal to 0. Another popular way of calculating the solution path is to use an adaptive tuning parameter sequence, which is defined as the locations where the active set changes (e.g., R packages lars, glmpath and plus). Hence, in S2, the tuning parameter sequences for sub-samples also have two respective packages (e.g. glmnet, glmpath, lars) that generate decreasing and increasing sequences, respectively. And in S3, the averaging is performed over the same tuning parameter or the same position on the solution path, respectively.

Without specifying the path generating method, we use $k$ as the index for averaging. Suppose the loss function employed in S2 is the negative log-likelihood; that is, for each $\lambda_k$ or model $\alpha_k$, the goal is to minimize

$$
\Gamma_k = E_s \left[ \frac{1}{n_v} (y_s' \hat{\theta}_{s^*,k} + 1'b(\hat{\theta}_{s^*,k})) \right],
$$

where $y_s = (y_i, i \in s)'$, $\hat{\theta}_{s^*,k} = (x_i'\hat{\beta}_{s^*,k}, i \in s)'$ with $\hat{\beta}_{s^*,k}$ as the estimator constructed by the sample $s^*$, and the expectation is taken with respect to the collection of all possible $\binom{n}{n_v}$ splits. For any vector $v \in \mathbb{R}^m$, let $b(v) = (b(v_1), \cdots, b(v_m))'$, $\hat{b}(v) = (\hat{b}(v_1), \cdots, \hat{b}(v_m))'$ and $\hat{b}(v) = \text{diag}(\hat{b}(v_1), \cdots, \hat{b}(v_m))$. When $n_v$ is large, it is NP-hard to calculate all the different splits. Therefore, S2 takes the popular Monte Carlo approach by using the average of $r$ splits as an estimate for the loss function,

$$
\hat{\Gamma}_k = \frac{1}{rn_v} \sum_{s \in S} \left[ y_s' \hat{\theta}_{s^*,k} + 1'b(\hat{\theta}_{s^*,k}) \right],
$$

where $S$ is the collection of different splits.

Similar to Shao (1996), we use $\alpha \subset \{1, \cdots, p\}$ to represent the indices of the active set, denote by $A$ the collection of all candidate models, and divide $A$ into two disjoint subsets: “correct” models $A_*$ and its complement $A \setminus A_*$, where

$$
A_* = \{ \alpha \in A : x'_n \beta_\alpha = x' \beta \},
$$

with $\beta_\alpha = (\beta_j, j \in \alpha)'$ and $x_n = (x_j, j \in \alpha)'$. Define $X_\alpha = (x_{ij}, i = 1, \cdots, n; j \in \alpha)$. For models in $A_*$, the number of false negatives is 0 (FN = 0); and FN > 0 for models in $A \setminus A_*$. Here we give two definitions which constitute the fundamental concept of this paper.

**Definition 1.** (Optimal Model) We define optimal model as $\alpha_* \in A_*$, such that for all $\alpha \in A_*$ and $\alpha \neq \alpha_*$, $\|\alpha_*\|_0 < \|\alpha\|_0$. The model size of $\alpha_*$ is denoted as $d_*$. 

**Remark 1.** The existence of the optimal model entails that it is also unique.

**Definition 2.** (Tuning Parameter Selection Consistency) We say that a method has tuning parameter selection consistency property, if the selected model $\hat{\alpha}_n$ satisfies

$$
\lim_{n \to \infty} P(\hat{\alpha}_n = \alpha_*) = 1.
$$
Remark 2. If there are more than one models with size \( d_* \), the consistency concept for a tuning parameter selection method could be redefined as the chosen model lies in the optimal model set with probability tending to 1.

Remark 3. In the situation when the true model \( \mathcal{O} \) lies on the solution path, the definition guarantees that the tuning parameter selection method selects the true model with probability tending to one.

For each \( \alpha \in \mathcal{A} \), we define \( \hat{\beta}_\alpha \) as the corresponding penalized estimator of \( \beta_\alpha \); that is,

\[
\hat{\beta}_\alpha = \arg \min_{\beta_\alpha} \left[ -\ell_\alpha(y; \beta_\alpha) + \sum_{j \in \alpha} \rho(\|\beta_j\|; \lambda, \gamma) \right],
\]

where \( \ell_\alpha(y; \cdot) \) is the log-likelihood function restricted on the subspace indexed by \( \alpha \), i.e., \( x_{\alpha,i} \) is used instead of \( x_i \). Similarly, we denote the maximum likelihood estimator (MLE) and the restricted MLE with respect to the index \( \alpha \) as \( \hat{\beta} \) and \( \hat{\beta}_\alpha \), respectively. For this model evaluation scenario, \( k \) in (3) is replaced by \( \alpha \), and \( \Gamma_\alpha \) is defined correspondingly. By plugging \( \hat{\beta}_\alpha \) and \( \hat{\beta}_\alpha \) into (4), \( \hat{\Gamma}_\alpha \) and \( \hat{\Gamma}_\alpha \) are defined, respectively.

In this paper, \( \hat{\Gamma}, \hat{\Gamma}, \hat{\beta}_\alpha, \hat{\beta}_\alpha \) all depend on the sample size \( n \), but to keep notations simple, we omit the subscript \( n \). When talking about asymptotic behavior, it always implies that \( p \to \infty \) as \( n \to \infty \).

2.3 Conditions

In this section, we list the major conditions needed in this paper.

**Condition 1.** (Candidate Set Condition) The optimal model \( \alpha_* \in \mathcal{A}_c \) exists. Denote by \( N = \| \mathcal{A} \|_0 \) the total number of candidate models and \( N_c = \| \mathcal{A}_c \|_0 \) the number of correct models. Denote \( d_{\text{max}} = \max_{\alpha \in \mathcal{A}_c} \| \alpha \|_0 \), \( d_* = \max\{ d_{\text{max}} - d_*, d_* \} \). The following hold: \( n_c d_* < n \), \( N_c > 0 \), and

\[
N = o \left( \exp \left( \frac{n}{n_c d_*} \right) \right). \tag{5}
\]

Condition 1 assures the candidate set is well behaved. The possible size of the candidate set \( N \) can diverge at the rate in (5). This condition also requires the upper bound of the sizes of the correct models. We allow the correct model sizes diverge as long as \( n_c d_* < n \).

Note that the commonly used path algorithms (e.g., glmnet) usually yield a fixed number of models, which trivially satisfies the condition. In addition, we assume the existence of the optimal model.

**Condition 2.** (GLM Condition)

(1a). \( b(\cdot) > 0 \) has continuous first, second and third order derivatives \( \dot{b}(\cdot), \ddot{b}(\cdot) \) and \( \dddot{b}(\cdot) \). In addition, \( \dddot{b}(\cdot) > 0 \).
(1b). For deterministic \( x_i \), \( \sup_i \|x_i\| < \infty \); for random \( x_i \), there exists a function \( h(\cdot) \) and \( \epsilon_0 > 0 \) such that for any \( \alpha \in A_c \) and \( \eta_{\alpha} \in \{ \eta_{\alpha} : \| \eta_{\alpha} - \beta_{\alpha} \| \leq \epsilon_0 \} \), we have
\[
E[h(x)] < \infty, \; E[h_{\alpha}(x_\alpha)] < \infty, \; E[\| h(x_{\alpha}) \|_2^2] \leq h_{\alpha}(x_{\alpha}), \; \text{and} \; E[\| h(x_{\alpha}) \|_2^2] \leq h_{\alpha}(x_{\alpha}) \] where \( h_{\alpha} \) is the function \( h \) restricted to the subspace spanned by \( x_{\alpha} \).

This is a common condition for generalized linear models, which has similar spirit as Condition C3 in Shao (1996).

**Condition 3.** (Invertibility Condition) \( \text{IC}(c_*, q^*) \): There exist \( c_* > 0 \) and \( q^* = \Theta(\sqrt{n/p}) \), such that \( \forall A \subset \{1, \ldots, p\} \) with \( \|A\|_0 = q^* \geq d_* \geq d_0 \), and for any \( \eta_A \in \{ \eta_A : \| \eta_A - \beta_A \| \leq \epsilon_0 \} \), where \( \epsilon_0 > 0 \) is fixed, and if \( v \) is a \( q^* \)-dimensional vector, we have, for deterministic \( x_i \),
\[
0 < c_* \leq \frac{\| (b(X_A \eta_A))^{1/2} X_A v \|}{\sqrt{\|v\|^2}} < \infty;
\]
for random \( x_i \),
\[
P \left\{ c_* \leq \frac{\| (b(X_A \eta_A))^{1/2} X_A v \|}{\sqrt{\|v\|^2}} \right\} \to 1.
\]

Here, for \( g_1(n) \) and \( g_2(n) \), \( g_1(n) = \Theta(g_2(n)) \) means there exist positive constants \( c_1 \) and \( c_2 \), such that \( c_1 \leq \liminf_n g_1(n)/g_2(n) \leq \limsup_n g_1(n)/g_2(n) \leq c_2 \). Correspondingly, \( \Theta_p(\cdot) \) represents the notation when the previous chain of inequalities holds in probability tending to 1.

This condition indicates that in any manifold of dimension less than or equal to \( q^* \), its corresponding MLE is well-defined and unique. Notice this is a weaker version of the Sparse Riesz Condition (Zhang and Huang, 2008). With the Invertibility Condition, we can safely terminate our calculation (to be specified below) when the current model size exceeds \( q^* \), without the risk of missing the optimal model.

**Condition 4.** (Beta-Min Condition) For the true model \( \mathcal{O} \), we assume
\[
\beta_* \equiv \min_{j \in \mathcal{O}} |\beta_j| \gg \sqrt{\frac{\log p}{n}}.
\]

This is a common condition in the high-dimensional sparse recovery literature, which guarantees the signals are detectable from the noises. If \( p = O(\exp(n^a)) \), with \( 0 < a < 1 \), then \( \beta_* = \Theta(1) \) is sufficient to satisfy this condition. Generally speaking, \( \beta_* \) can go to zero slowly as \( n \) diverges, so it is mild and reasonable.

**Condition 5.** (Design Matrix Condition) For all \( A \subset \{1, \ldots, p\} \) with \( |A| = q^* \), where \( q^* \) is the constant from Condition 3, and for any \( \eta_A \in \{ \zeta_A : \| \zeta_A - \beta_A \| \leq \epsilon_0 \} \), where \( \epsilon_0 > 0 \) is fixed, the following is satisfied,
\[
\lim_{n \to \infty} \max_{s \in S} \left| \frac{1}{n} X_{s,A} b(x_{s,A} \eta_A) X_{s,A} - \frac{1}{n} X_{s',A} b(x_{s',A} \eta_A) X_{s',A} \right| = o_p(1),
\]
where the norm here is the operator norm of a matrix and \( S \) is the collection of splits.
Unless otherwise stated, the matrix norm used in this paper refers to the operator norm. Here, the collection $S$ can be different across scenarios, which will be clarified in the subsequent sections. This condition bounds the difference between the Fisher information of the validation set and the construction set. This is a reasonably weak condition, the technical details of its resemble version in linear regression is studied in Section 4.4 of Shao (1993).

To investigate the correlation structure in the random design case, we borrow the idea from Zhang and Huang (2008) and formulate the problem as relationship between a response variable $Y$ and infinitely many possible covariates $\{\xi_k, k = 1, 2, \cdots\}$. Each sample is collected from the dependent variable $Y$ and $p$ covariates, and we have $n$ independent copies $(y^{(n)}_{i}, x^{(n)}_{ij}, j = 1, \cdots, p)$ of the random vector $(Y, \xi_{k_j}, j = 1, \cdots, p)$ for certain $k_1 < \cdots < k_p, p \equiv p^{(n)}$. In what follows, the superscript $(n)$ is often omitted, and the correlation condition will be naturally imposed on the stochastic process $\{\xi_i, i \geq 1\}$.

**Condition 6.** (Correlation Condition) For deterministic $x_i$’s, denote the sample correlation as $r_{ij} = \frac{x_i'x_j}{n}$. For random $x_i$’s, suppose that the $n$ rows of a random matrix $X_{n \times p}$ are i.i.d. copies of a subvector $(\xi_{k_1}, \cdots, \xi_{k_p})$ of $\{\xi_j, j \geq 1\}$, where $\{\xi_j, j \geq 1\}$ is a Gaussian process, with zero mean, unit variance and $\text{Corr}(\xi_i, \xi_j) = r_{ij}$. For both scenarios, $|r_{ij}| < \rho_{|i-j|}$ for $i \neq j$ with $\rho_m < 1$ and $\rho_m \log m \to 0$.

## 3 Asymptotic Behavior of Cross-Validation in High-Dimensional Settings

Researchers have realized that the usual cross-validation methods for selecting the tuning parameter on the solution path of the penalized likelihood estimator are usually too conservative in the sense that they often lead to over-selection. In this section, we would like to explore the underlying reasons for this phenomenon.

Recall the original idea of cross-validation is to evaluate different models and find out the best one according to their predictive performances on the validation set. However, in the problem of selecting the tuning parameter for high-dimensional penalized likelihood estimation, the method is changed to select a tuning parameter or the position of the model on the solution path. But due to the data-driven property of the penalized estimators, the theoretical results are intractable when the sequence of models are different for different splits, when the same tuning parameters are used. In this section, we assume the model sequences of different splits are the same, which enables us to focus on the shrinkage effect and the choice of $n_c$.

### 3.1 Shrinkage Effect

Nowadays researchers hold a not-yet-proven belief, that the underlying reason for the over-selection problem in the cross-validation based Lasso estimator is the shrinkage effect from the Lasso penalty. In this subsection, we will show asymptotically, this is not always true. For simplicity, we convey the idea via the Lasso penalized linear regression. In addition, we assume the active set sequences are exactly the same for
different splits. This enables us to concentrate on the possible problems caused by the shrinkage. First, we give a lemma on the asymptotic behavior of two order statistics, which has interests on its own. The proof is relegated to the appendix.

**Lemma 1.** Assume \( \{S_i, i \geq 1\} \) is a Gaussian process, and can be decomposed as \( S_i = \eta_i + m_i \), where \( \{\eta_i, i \geq 1\} \) is a Gaussian process with zero mean, unit variance and correlations \( \rho_{ij} \) such that \( |\rho_{ij}| < \rho_{|i-j|} \) for \( i \neq j \) with \( \rho_k < 1 \) for all \( 1 \leq k \leq p \), and \( \rho_p \log p \to 0 \). Assume

\[
\max_{1 \leq i \leq p} |m_i| = o((\log p)^{1/2}), \quad \text{as } p \to \infty.
\]

Define \( T_k \) and \( T_\ell \) as the order statistics \( |S|_{(p-k)} \) and \( |S|_{(p-\ell)} \), respectively, where \( k \) and \( \ell \) are fixed integers with \( 2 \leq \ell < k < p \). Then,

\[
\lim_{p \to \infty} P\{kT_k^2 > \ell T_\ell^2\} = 1.
\]

With Lemma 1 in hand, we can investigate the shrinkage effect by decomposing the negative log-likelihood from S2 of Algorithm 1 (in Section 2) into the restricted MLE part and the shrinkage effect part. The results are summarized in the following Proposition.

**Proposition 1.** Given \( n \) observations \( (x_i, y_i), i = 1, \cdots, n \), with \( y_i = x_i' \beta + \varepsilon_i \), where \( \varepsilon_i \overset{i.i.d.}{\sim} N(0, \sigma^2) \), assume the design matrix \( X = (x_1', \cdots, x_n')' \) is orthogonal with \( p < n \). Given a collection of candidate models \( A \) satisfying Condition 1, for each \( \alpha \in A \), we have the following expansion

\[
\hat{\Gamma}_\alpha = \hat{\Gamma}_\alpha + \lambda_\alpha^2 d_\alpha,
\]

where \( \lambda_\alpha \) is the corresponding tuning parameter for model \( \alpha \) from the Lasso estimator, and \( d_\alpha \) is the model size of \( \alpha \); \( \hat{\Gamma}_\alpha \) is the negative log-likelihood evaluated at the restricted MLE \( \hat{\beta}_\alpha \) of model \( \alpha \), which was defined in Section 2.2. Additionally, for each \( \alpha \in A \), with \( \alpha \neq \alpha_* \), we have

\[
\lim_{n \to \infty} P\{\lambda_\alpha^2 d_\alpha < \lambda_{\alpha_*}^2 d_*\} = 0.
\]

**Proof.** Recall the KKT conditions of Lasso penalized linear regression,

\[
\begin{cases}
\frac{1}{n} x_j' (y - X_\alpha \hat{\beta}_\alpha) = \lambda_\alpha \text{sgn}(\hat{\beta}_j), & \hat{\beta}_j \neq 0; \\
\frac{1}{n} x_j' (y - X_\alpha \hat{\beta}_\alpha) \leq \lambda_\alpha, & \hat{\beta}_j = 0.
\end{cases}
\]

Then, (6) can be easily derived by noticing the fact that for orthonormal design, \( \hat{\beta}_\alpha = \hat{\beta}_\alpha - \lambda_\alpha \text{sgn}(\hat{\beta}_\alpha) \).

In the orthonormal design, \( |x_j (y - X \hat{\beta})| = |\beta_j - \hat{\beta}_j + x_j' \varepsilon / n| \). When \( \lambda \) decreases from \( \infty \) to 0, covariates are selected in the descending order of \( |\beta_j + x_j' \varepsilon / n|, j = 1, \cdots, p \). For correct models, \( \lambda = \max_{j \in \{1, \cdots, p\} \setminus \alpha_*, \alpha \in A} |x_j' \varepsilon / n| \).

For a sequence of random variables \( \{W_1, \cdots, W_M\} \), denote \( W_{(m:M)} \) as the \( m \)-th maximum order statistics among \( M \) random variables. Here, we use both the indices
and $M$ to emphasize that the total number of variables is increasing. Hence, define $Z_j = x'_j \varepsilon / n$, $\lambda_\alpha = |Z|_{(p-d_\alpha:p-d_\alpha)}$, and for $\alpha \in A_c$, $\lambda_\alpha = |Z|_{(p-d_\alpha:p-d_\alpha)}$. Then, applying Lemma 1, (7) holds.

From Proposition 1, we can see that in the orthonormal design case, the extra shrinkage term from the Lasso penalty actually helps the model selection asymptotically, which is opposite to the empirical evidence researchers have observed. We will study this “contradiction” in the next subsection when the consistency of the $\text{CV}(n_v)$ is studied. As will be clarified in Theorem 1, if $\text{CV}(n_v)$ is consistent for using the restricted MLE as the estimator for calculating the criterion function $\tilde{\Gamma}_\alpha$, it will also be consistent for the Lasso penalized estimator.

3.2 Asymptotic behavior of $\text{CV}(n_v)$

Now the problem is narrowed down to the restricted MLE. Define $\mu = \lim_{n \to \infty} n_c / n$, with $0 \leq \mu \leq 1$. In Shao (1993), the author proved that in order to achieve a consistent selection for the restricted MLE, $\mu = 0$ is a sufficient condition. In particular, K-fold cross-validation is not consistent. In the following theorem, we show a surprising result that $\text{CV}(n_v)$ is consistent even when $\mu > 0$, thanks to the shrinkage effect.

**Theorem 1.** For the linear regression models, we consider the solution path generated using Lasso. Assume $n_c \to \infty$ as $n \to \infty$, and the model sequences are the same across all splits. When Conditions 7 - 8 are satisfied, and the number of the splits $r$ satisfies $r^{-1} n_c^{-2} n^2 \to 0$, $\text{CV}(n_v)$ is consistent.

Noteworthy, we did not list $p$’s order as a condition in the theorem. Recall that our starting point is an available collection of candidate models, which is usually the output of a certain path algorithm. Since we require Condition 1 hold, for different path algorithms, different $p$’s order and corresponding technical details are needed. To make our contribution prominent, we omit all the details and refer the interested readers to the literature listed in the introduction. For example, if `plus` is used, $p = O(\exp(n^a))$, $0 < a < 1$, is allowed.

Here, we will provide a sketch of the important parts of the proof, while the details can be found in the Appendix. From (13) in the Appendix,

$$
\hat{\Gamma}_\alpha = \Delta_{\alpha,n} + \frac{1}{n} \varepsilon' \varepsilon + \frac{1}{n_c} d_\alpha \sigma^2 - \frac{1}{n} \varepsilon' P_\alpha \varepsilon + o \left( \frac{1}{n_c} \right) + \lambda_\alpha^2 d_\alpha (1 + o(1)) \\
\equiv \hat{\Gamma}_\alpha + \lambda_\alpha^2 d_\alpha (1 + o(1)),
$$

where $\Delta_{\alpha,n} = \frac{(1/n)\beta' X' (I_n - P_\alpha) X \beta}{n}$. As shown in the Appendix, $\Delta_{\alpha,n} > 0$ for $\alpha \in A \setminus A_c$, then it follows from Gaussian concentration inequality (Lalley, 2013) that $P\{\hat{\alpha} \notin A \setminus A_c\} \to 1$.

For $\alpha \in A_c$, no matter how large $\mu$ is, the dominating term of $\hat{\Gamma}_\alpha$ is $\lambda_\alpha^2 d_\alpha$. Combining the results in Lemma 1 it is shown that the model selection is consistent using CV($n_v$).
Figure 1: The left panel shows the ratio of the $\lambda_\alpha$ sequence derived from glmnet to their corresponding theoretical expectations, and the right panel shows the value of $\lambda^2_\alpha d_\alpha$, where $\alpha \in \{\alpha \in A_c : \text{FP of } \alpha \text{ is larger than 0}\}$.

In practice, however, we observe that even for the orthonormal design when $p < n$, the value of $\lambda_\alpha$ is systematically smaller than the theoretical order when a majority of noise variables are included. The possible reason is that the convergence rate of the maximum of Gaussian random variables to the Gumbel distribution is very slow, which leads to a smaller magnitude of the $\lambda_\alpha$ when the active set is large. This implies, instead of the theoretical approximation that $\lambda_\alpha \approx \sigma \sqrt{2 \log (p - d_\alpha) / n_c}$ (see the proof of Lemma 1 in Section 8.1) and (7), $\lambda^2_\alpha d_\alpha$ cannot dominate the other terms when the active set is large. In practice, it also suffers from the different $\lambda$ sequences yielded by different subsamples (details can be found in Section 5.1). Whence, we turn into detailed discussion of $\hat{\Gamma}_{\alpha 1}$.

If $\mu > 0$, then for $\alpha \in A_c$ with $\alpha \neq \alpha_\ast$, we have

$$\lim_{n} P\{\hat{\Gamma}_{\alpha 1} < \hat{\Gamma}_{\alpha \ast 1}\} = P \left\{ \frac{1}{\mu} (d_\alpha - d_\ast) < \varepsilon' (P_\alpha - P_{\alpha_\ast}) \varepsilon \right\} = P \{ k / \mu < \chi^2(k) \} > 0,$$

where $d_\alpha - d_\ast = k$. As a result, the model selection is likely to be inconsistent in practice.

However, if $\mu = 0$, then we have

$$\hat{\Gamma}_{\alpha 1} = \frac{1}{n} \varepsilon' \varepsilon + \frac{1}{n_c} d_\alpha \sigma^2 + o \left( \frac{1}{n_c} \right),$$
where $\hat{\Gamma}_{\alpha 1}$ increases when noise variables are activated, i.e., the model selection is consistent if we use $\hat{\Gamma}_{\alpha 1}$ as the criterion function.

From the above observation, we advocate the use of $\text{CV}(n_v)$ with $\mu = 0$, which will be described in detail in the next subsection.

To demonstrate the issue of the shrinkage in finite samples, we show a toy simulation example for variable selection in high-dimensional linear regression using the Lasso penalty. The simulation setup is taken to be the same as in Example 1(i) with $\rho = 0$ (see Section 5 for a detailed description) with the results summarized in Figure 4. Notice that we only report the part of the solution path where noise variables are involved ($\text{FP} > 0$). The left panel shows the ratio of actual $\lambda$ values to their corresponding theoretical expectations. It is clear that as more noise variables are included in the model, the quality of the approximation deteriorates very quickly. The right panel shows how $\lambda^2 d_\alpha$ changes on the solution path. In the early stage when a few noise variables are included, the values of $\lambda^2 d_\alpha$ increase as $d_\alpha$ increases, which verifies the result of Lemma 1. However, when too many noise variables are included, the relationship takes the opposite direction for which we conjecture the partial reason to be the violation of the correlation condition in Lemma 1.

There are two possible generalizations of the theorem. One is to extend linear regression to the generalized linear models framework. We conjecture the consistency still holds, but it may require additional efforts on studying the limiting distribution of the order statistics. The other possible generalization is to extend Lasso penalty to folded-concave penalties. Again, we conjecture the same result holds. The complication for folded-concave penalties lies on the uncertainty of the shrinkage level for different variables, i.e., if a variable is selected, the shrinkage imposed could be any value between 0 and the current $\lambda$. We will show some simulation results for both generalizations while leaving the rigorous treatment as future work.

3.3 Summary

We have now discussed some potential problems with the traditional cross-validation method. It is shown that the shrinkage effect is not always the reason of over-selection, while the choice of $n_v$ is critical for the success of variable selection. In light of this, we propose the following leave-$n_v$-out cross-validation (CV($n_v$)) algorithm.

Algorithm 2. (CV($n_v$))

S1. For the whole dataset, find a decreasing sequence of tuning parameters $\lambda = (\lambda_1, \lambda_2, \cdots, \lambda_N)$, which is usually equal spaced in log-scale and $\lambda_1$ is the minimum tuning parameter which will produce the solution $\hat{\beta} = 0$. Compute the solution path with the tuning parameter sequence $\lambda$ and the corresponding sequence of solutions is denoted as $\hat{\beta}(\lambda) = (\hat{\beta}(\lambda_1), \hat{\beta}(\lambda_2), \cdots, \hat{\beta}(\lambda_N))$.

S2. Randomly split the whole dataset into $\{(x_i, y_i), i \in s\}$ (the validation set) and $\{(x_i, y_i), i \in s^c\}$ (the construction set) $r$ times, where $s$ is a subset of $\{1, \cdots, n\}$ containing $n_v$ integers and $s^c$ is its complement containing $n_c$ integers, with $n_v/n \to 0$ and $n_c \to \infty$ as $n \to \infty$. For each split $j = 1, \cdots, r$, compute the solution path $\hat{\beta}^{(j)}(\lambda)$ for the construction data in $s^c$ using the same tuning pa-
rameter sequence λ from S1. Then, compute the loss function (e.g., negative log-likelihood) on the validation data in s with the solution path $\hat{\beta}^{(j)}(\lambda)$.

S3. Average the loss function over r splits for each tuning parameter on the solution path, and then choose the one with the smallest average loss, say $\hat{\lambda}$. From the sequence of solutions $\hat{\beta}(\lambda)$ in S1, pick the solution with $\hat{\lambda}$.

S4. Compute the restricted MLE for the model corresponding to the solution in S3.

As will be shown in the simulation studies, CV($n_v$) has competitive performance in terms of both model selection and prediction. Theorem 1 showed the consistency of CV($n_v$) under the strong assumption that the model sequences are the same across all different splits, which is rarely true in the real world examples. Due to the complication arising from different model sequences generated from the same sequence of tuning parameters λ, we conjecture that strong conditions on the design matrix are needed to guarantee the model selection consistency.

4 Consistent Cross-Validation

In Section 3, we proposed CV($n_v$) in Algorithm 2 whose theoretical results were provided under relatively strong conditions. In this section, we propose a new tuning parameter selection method, Consistent Cross-Validation (CCV), which avoids the problems of the alignment of the model sequence and the shrinkage effect. We will show the CCV is consistent under mild technical conditions under the generalized linear model framework for both convex and folded-concave penalty functions. An efficient algorithm for the CCV is presented as follows.

Algorithm 3. (Consistent Cross-Validation)

S1. Compute the solution path with the whole dataset. A sequence of solutions $\hat{\beta}(\lambda)$ is generated with corresponding penalty level λ. Along the path, a sequence of active sets are determined.

S2. Randomly split the whole dataset into construction dataset $s_c$ (size $n_c$) and validation dataset $s$ (size $n_v$) r times, with $n_c/n \to 0$ and $n_c \to \infty$ as $n \to \infty$. Compute the restricted MLE path for each split according to the active set sequence generated in S1.

S3. Average the negative log-likelihood over r splits for each active set in S1, and choose the active set $\hat{\alpha}$ with the smallest average value.

S4. Compute the restricted MLE for the selected model $\hat{\alpha}$ in S3.

The main idea of the algorithm is to use the whole dataset for deriving the solution path and the corresponding active set sequence. The problem of selecting the tuning parameter is then reduced to the choice of the best active set. Condition 3 guarantees that the restricted MLE needed in S2 can be calculated for models up to size $q^*$, which includes the optimal model. In this sense, we recast the tuning parameter selection problem for high-dimensional generalized linear models to the problem of model selection of a low-dimensional generalized linear models.
Theorem 2. For the penalized generalized linear models with separable penalties, assume Conditions 1-5 hold with \( n_c/n \to 0, n_c \to \infty \), and the number of the splits \( r \) satisfies
\[
r^{-1}n_c^{-2}n^2 \to 0.
\]
Then, the CCV is a consistent tuning parameter selection method.

Similar to Theorem 1, we did not list the order of \( p \) as a condition. But high-dimensional setting such as \( p = O(\exp(n^a)) \), \( 0 < a < 1 \) is allowed, as long as Condition 4 satisfied. Theorem 2 can be easily derived from Lemma 3 (Section 8.4) by noticing the fact that the CCV algorithm narrows the potentially high-dimensional problem down to a low-dimensional \( (d < n) \) one. With the selection consistency at hand, S4 in Algorithm 3 is applied to improve the estimation and the prediction performance.

It is worth to point out that \( n_c \) appears in both CV(\( n_v \)) and the CCV algorithm. Comparing steps S2 of both algorithms, we notice that after getting a solution path for the whole dataset, different methods are used to construct paths for sub-samples. For CV(\( n_v \)), similar penalized solution paths are constructed, which remains a high-dimensional problem; while the CCV solves a low-dimensional problem. Therefore, compared with CV(\( n_v \)), a smaller \( n_c \) is needed for CCV to keep the estimation process stable. For CCV, we have more data available for validation, thereby making the detection of the differences among different models easier. This phenomenon will be verified numerically in the next section. Another remark is that although the consistency holds for both convex penalty (e.g., Lasso) and the folded-concave penalties (e.g., SCAD and MCP), the final performance of the method depends on the quality of the active set sequence derived in S1.

5 Simulation

In this section, we conduct simulations to assess the performance of the proposed CV(\( n_v \)) and CCV methods in terms of model selection consistency and prediction.

5.1 Coherent Rate

Suppose the sequence of tuning parameters of the whole dataset is \( \lambda = (\lambda_1, \cdots, \lambda_N) \). Denote \( \alpha^{(j)}_\ell \) as the active set of the \( \ell \)-th estimate on the path constructed by sub-sample \( s_j \) using the same tuning parameter sequence \( \lambda \), where \( \ell = 1, \cdots, N; j = 0, 1, \cdots, r \), and \( s_0 \) represents the whole dataset. We define the coherent rate (CR) as a sequence representing the degree of agreement of the active sets across different splits for each tuning parameter location,
\[
\text{CR}(\ell) = \#\{ j : \alpha^{(j)}_\ell = \alpha^{(0)}_\ell \}/r, \text{ where } \ell = 1, \cdots, N.
\]
In the ideal case when CR(\( \cdot \)) equals 1 for all \( \ell \)'s, the classical cross-validation method for choosing the tuning parameter serves as an excellent surrogate for selecting the optimal model. However, this is rarely true in practice, especially when the noise variables are activated in the estimators. We demonstrate the behavior of the CR as follows.
Example 1. (i) Linear regression. For \( i = 1, \cdots, n \), we generate the response \( y_i \) as 
\[
y_i = x_i' \beta + \epsilon_i,
\]
where \( x_i \sim N(0, \Sigma) \) with \( 0_p \) the length-\( p \) vector with 0 entries and \( \Sigma_{j,k} = \rho^{|j-k|}, \epsilon_i \sim N(0, 1) \), \( \rho = 0.5 \), \( (n, p) = (500, 1000) \) and \( \beta \in \mathbb{R}^p \) with the first 5 coordinates \( (2.0, 1.6, 1.2, 0.8, 0.4) \) and 0 elsewhere. (ii) Logistic regression. For \( i = 1, \cdots, n \), we generate the response \( y_i \) as 
\[
P(y_i = 1) = \frac{\exp(x_i' \beta)}{1 + \exp(x_i' \beta)},
\]
where \( \beta \in \mathbb{R}^p \) with the first 5 coordinates \( (3.0, 1.5, 0.0, 2.0) \) and 0 elsewhere. The remaining part of the simulation setting is the same as in (i). For each setting, we do 10-fold cross-validation 100 times.

We calculate the solution paths using the R package glmnet for Lasso, and the R package ncvreg for SCAD and MCP. Figure 2 shows how the CR changes along the path in different scenarios. In addition, we mark the location of the 10-fold CV chosen estimator and the first location where noise variables are selected. It is obvious the CR is much smaller than 1 in a majority of locations after the noise variables are selected. It is interesting to compare the behavior for different penalty functions as well as for different models. For linear regression, the CR is close to 1 at the 10-fold CV chosen location for both SCAD and MCP penalties, while it is close to 0 for Lasso penalty. For logistic regression, all penalties lead to a very small CR even before the noise variables are selected.

From the path-generating procedure, estimators can be regarded as functions of the tuning parameter. Due to their one-to-one correspondence, tuning parameters can also be regarded as functions of estimators, given the data. So the phenomenon we noticed above is due to the data-driven property of tuning parameters selection. When the data are changed from whole sample to different subsample splits, same tuning parameter sequence yields different estimator sequences. If one wants to hold the estimators (or at least the models) the same, very stringent conditions should be imposed on the design matrix, which are usually not satisfied even for the simple simulation settings we have shown.

5.2 Linear Regression

For linear regression, we use the same setting as Example 1 (i) with \( \rho = 0 \) and \( \rho = 0.5 \), and repeat the simulation 100 times. For SCAD and MCP paths, we use the default \( \gamma = 3 \) in the ncvreg package. In Table 4 for CV(\( n_v \)), we set \( n_v = \lceil n^{2/3} \rceil = 63 \) and \( n_v = n - n_c = 437 \); for CCV, we set \( n_v = \lceil n^{1/2} \rceil = 23 \) and \( n_v = n - n_c = 477 \). We compare our results with \( K \)-fold cross-validation in glmnet and ncvreg, with the default \( K = 10 \). As suggested by an anonymous referee, we also include the comparison with \( K \)-fold CV with 1SE rule, where the \( \lambda \) is chosen as the one with the minimum loss function value plus one standard error (1SE), rather than the one corresponding to the minimum loss function value as used in regular \( K \)-fold CV. To compare these methods, we report false negative (FN), false positive (FP) and prediction error (PE). Here, the PE is the average prediction error evaluated at an independent test dataset of size \( n \).

In Table 4 for Lasso penalty, \( K \)-fold CV has the largest mean FP followed by CV(\( n_v \)) and 1SE, and CCV performs the best in both \( \rho = 0 \) and \( \rho = 0.5 \) cases. For prediction error, CV(\( n_v \)) and CCV have almost the same performance, outperforming \( K \)-fold CV and 1SE.
Figure 2: Coherent Rate along the path for Lasso, SCAD and MCP penalized linear and logistic regression estimators, respectively. The solid line “—” is where 10-fold CV chooses, and the dashed line “— —” is where noises start to get involved.
Table 1: Comparison of CV($n_v$), CCV and K-fold CV ($K = 10$), for $\rho = 0$ and $\rho = 0.5$ cases. Results are reported in the form (mean (standard deviation)). For CV($n_v$) and CCV, $n_v = \lceil \sqrt[3]{n} \rceil$ and $n_c = \lceil \sqrt{n} \rceil$, respectively. $r = 50$ splits and 100 repetitions.

<table>
<thead>
<tr>
<th>Models</th>
<th>$\rho = 0$</th>
<th>$\rho = 0.5$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>FN</td>
<td>FP</td>
</tr>
<tr>
<td>CV($n_v$)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Lasso</td>
<td>0.00(0.00)</td>
<td>0.11(0.37)</td>
</tr>
<tr>
<td>SCAD</td>
<td>0.00(0.00)</td>
<td>0.00(0.00)</td>
</tr>
<tr>
<td>MCP</td>
<td>0.00(0.00)</td>
<td>0.07(0.26)</td>
</tr>
<tr>
<td>CCV</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Lasso</td>
<td>0.00(0.00)</td>
<td>0.00(0.00)</td>
</tr>
<tr>
<td>SCAD</td>
<td>0.00(0.00)</td>
<td>0.01(0.10)</td>
</tr>
<tr>
<td>MCP</td>
<td>0.00(0.00)</td>
<td>0.02(0.14)</td>
</tr>
<tr>
<td>K-fold</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Lasso</td>
<td>0.00(0.00)</td>
<td>29.16(19.33)</td>
</tr>
<tr>
<td>SCAD</td>
<td>0.00(0.00)</td>
<td>4.71(6.36)</td>
</tr>
<tr>
<td>MCP</td>
<td>0.00(0.00)</td>
<td>2.45(4.28)</td>
</tr>
<tr>
<td>1SE</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Lasso</td>
<td>0.00(0.00)</td>
<td>0.02(0.01)</td>
</tr>
<tr>
<td>SCAD</td>
<td>0.01(0.10)</td>
<td>0.02(0.14)</td>
</tr>
<tr>
<td>MCP</td>
<td>0.01(0.10)</td>
<td>0.01(0.10)</td>
</tr>
</tbody>
</table>

SCAD and MCP penalty cases have similar behavior. The FP’s of K-fold CV for them are not as large as they are in the Lasso cases, but CV($n_v$) and CCV still outperform K-fold CV along with the ISE rule in terms of both variable selection and prediction. But it is worth to point out that the difference is not as significant as that in the Lasso case, due to the asymptotic unbiasedness property of SCAD and MCP. From the FN results, 1SE is aggressive when $\rho = 0.5$.

Although CV($n_v$) and CCV appear to have similar behavior, different $n_c$ rates are applied. We will conduct a systematic study on how the $n_c$ rates affect the performance in Section 5.4. We will show that in general, compared to CCV, CV($n_v$) needs a larger size for the construction dataset to make the algorithm stable.

We also present the comparisons of the values of the universal thresholding and the $\lambda$ values from different methods in Table 2. Due to the complexity caused by correlation when computing the universal thresholding, we only consider the uncorrelated design ($\rho = 0$). As expected, the $\lambda$ values chosen by CCV and CV($n_v$) are universally larger than those of K-fold and 1SE. The rationale of universal thresholding is the upper bound of the maximum of all the errors. Hence it can be regarded as a theoretical lower bound of $\lambda$ to remove all the noise variables. On the other hand, the selected $\lambda$ value should not exceed the minimum signal (0.4 in this example). Due to this, Table 2 also provides some rationale of the good performances of CCV and CV($n_v$).

### 5.3 Logistic Regression

For logistic regression, we use the same setting as Example 1 (ii) with $\rho = 0$ and $\rho = 0.5$, and repeat the simulation 100 times. In Table 3 for CV($n_v$) and CCV, we set $n_c = \lceil n^{3/4} \rceil = 106$ and $n_c = \lceil n^{2/3} \rceil = 63$, respectively. Different from linear case, instead of reporting prediction error, we report classification error (CE), which
Table 2: Comparison of λ values derived from various methods and the theoretical universal thresholding (Universal). Results are presented in the form of mean (standard deviation).

<table>
<thead>
<tr>
<th>n</th>
<th>Universal</th>
<th>CV($n_v$)</th>
<th>CCV</th>
<th>K-fold</th>
<th>1SE</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>0.21</td>
<td>0.22(0.04)</td>
<td>0.43(0.06)</td>
<td>0.12(0.02)</td>
<td>0.19(0.02)</td>
</tr>
<tr>
<td>500</td>
<td>0.17</td>
<td>0.20(0.02)</td>
<td>0.31(0.03)</td>
<td>0.09(0.01)</td>
<td>0.15(0.01)</td>
</tr>
</tbody>
</table>

Table 3: Comparison of CV($n_v$), CCV and K-fold CV ($K = 10$), for $\rho = 0$ and $\rho = 0.5$ cases. Results are reported in the form of mean (standard deviation). For CV($n_v$) and CCV, $n_c = \lceil n^{3/4} \rceil$ and $n_c = \lceil n^{2/3} \rceil$, respectively.

<table>
<thead>
<tr>
<th>Models</th>
<th>CV($n_v$)</th>
<th>$\rho = 0$</th>
<th>$\rho = 0.5$</th>
<th>$\rho = 0.5$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>FN</td>
<td>FP</td>
<td>CE(%)</td>
<td>FN</td>
</tr>
<tr>
<td>Lasso</td>
<td>0.00(0.00)</td>
<td>3.24(3.78)</td>
<td>10.96(0.01)</td>
<td>0.00(0.00)</td>
</tr>
<tr>
<td>SCAD</td>
<td>0.00(0.00)</td>
<td>0.32(0.66)</td>
<td>11.40(0.60)</td>
<td>0.00(0.00)</td>
</tr>
<tr>
<td>MCP</td>
<td>0.00(0.00)</td>
<td>0.04(0.20)</td>
<td>11.37(0.01)</td>
<td>0.00(0.00)</td>
</tr>
<tr>
<td>CV</td>
<td>FN</td>
<td>FP</td>
<td>CE(%)</td>
<td>FN</td>
</tr>
<tr>
<td>Lasso</td>
<td>0.00(0.00)</td>
<td>0.03(0.17)</td>
<td>11.38(0.51)</td>
<td>0.08(0.27)</td>
</tr>
<tr>
<td>SCAD</td>
<td>0.00(0.00)</td>
<td>0.03(0.17)</td>
<td>11.38(0.50)</td>
<td>0.08(0.27)</td>
</tr>
<tr>
<td>MCP</td>
<td>0.00(0.00)</td>
<td>0.03(0.17)</td>
<td>11.25(0.51)</td>
<td>0.19(0.39)</td>
</tr>
<tr>
<td>K-fold</td>
<td>FN</td>
<td>FP</td>
<td>CE(%)</td>
<td>FN</td>
</tr>
<tr>
<td>Lasso</td>
<td>0.00(0.00)</td>
<td>51.45(27.58)</td>
<td>11.83(1.17)</td>
<td>0.00(0.00)</td>
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<tr>
<td>SCAD</td>
<td>0.00(0.00)</td>
<td>15.77(12.10)</td>
<td>11.70(0.66)</td>
<td>0.00(0.00)</td>
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<tr>
<td>MCP</td>
<td>0.00(0.00)</td>
<td>2.97(5.39)</td>
<td>11.38(0.62)</td>
<td>0.00(0.00)</td>
</tr>
<tr>
<td>1SE</td>
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<td>FP</td>
<td>CE(%)</td>
<td>FN</td>
</tr>
<tr>
<td>Lasso</td>
<td>0.00(0.00)</td>
<td>8.73(10.25)</td>
<td>11.11(0.68)</td>
<td>0.00(0.00)</td>
</tr>
<tr>
<td>SCAD</td>
<td>0.00(0.00)</td>
<td>4.28(0.42)</td>
<td>11.23(0.48)</td>
<td>0.01(0.20)</td>
</tr>
<tr>
<td>MCP</td>
<td>0.00(0.00)</td>
<td>0.03(0.14)</td>
<td>13.79(0.78)</td>
<td>0.02(0.14)</td>
</tr>
</tbody>
</table>

is defined as the average classification error evaluated at an independent test dataset of size $n$. The remaining settings and packages used are the same as in the linear regression case. Here, we use a slightly larger $n_c$ for logistic regression due to the more stringent requirement on the sample size compared with linear regression.

In Table 3, CV($n_v$) and CCV significantly outperform K-fold CV in terms of FP. The difference is more significant than in the linear regression case, when SCAD or MCP penalty is used. For Lasso penalized logistic regression, 1SE rule has a significant number of FPs, compared with the linear regression case.

It is worth to note that, in the $\rho = 0.5$ case, the CCV has nonzero FN for all three cases. This is probably due to the correlation in the design matrix. We investigated the results and found that among these 100 repetitions, whenever there was a missing variable, CCV always missed $x_2$ which has the corresponding smallest absolute coefficient among the nonzero variables, and also has a high correlation with the first coordinate, which is the variable with the largest absolute value.

For the current $n_c$ settings, CV($n_v$) tends to be more conservative than CCV, with all zero FN, but larger FP. More discussions on the $n_c$ rate are available in the next subsection.
5.4 Order of $n_c$

As shown in Theorem 2, when $n_c/n \to 0$ and $\log p/n \to 0$, CCV is consistent. In this subsection, we study the performance when different $n_c$’s are used in the CV($n_v$) and CCV.

Here, we use the same settings as in Example 1, except we increase $p$ to 10,000. We display the results of CV($n_v$) and CCV in Figures 3 and 4, respectively. In each figure, different methods are presented, including 10-fold cross-validation, and CCV with $n_c = \lceil n^{1/2} \rceil, \lceil n^{7/12} \rceil, \lceil n^{2/3} \rceil, \lceil n^{3/4} \rceil$; for CV($n_v$), $n_c = \lceil n^{3/5} \rceil$ is also included. And for each setting, results of $n = 400, n = 700$ and $n = 1,000$ are showed; splitting times $r = 50$ and repetition times $N = 50$.

In these figures, we render the median of false positives and negatives as $n_c$ varies, and to make the comparison clearer, we set the false negatives as a negative value. For both linear and logistic regression models, the larger the order of $n_c$ is, the more false positives are involved, but the less false negatives. The trend for different $n$ is not obvious.

In CCV, for linear regression cases, $n_c = \lceil n^{1/2} \rceil$ has the best performance, while $n_c = \lceil n^{2/3} \rceil$ is the best for logistic regression, which are highlighted in red in each setting. Under the canonical link, the Fisher information for GLM can be written as $1/a(\phi) \cdot X'WX$, where $\phi$ is the dispersion parameter. For logistic regression, $W = \text{diag}\{\pi_1(1 - \pi_1), \ldots, \pi_n(1 - \pi_n)\}$, where $\pi_i = \exp(x_i'\beta)/(1 + \exp(x_i'\beta)) < 1$ in non-degenerate cases; while for linear regression, $W = I_n$. This indicates that logistic regression always has less information than linear regression, which leads to the fact that compared with linear regression, we need a larger sample size for the logistic regression to have the same level of estimation accuracy. This is also the reason we adopt such $n_c$ rates in the previous subsections. Another interesting observation is that for Lasso penalized models, the CCV improves a lot, while in the SCAD and MCP case, the improvement is not as significant.

For CV($n_v$), slightly larger $n_c$ is needed as expected. For linear regression, the best performance is attained when $n_c = \lceil n^{2/3} \rceil$, and for logistic regression, the best choice is $n_c = \lceil n^{3/4} \rceil$. We also included $n_c = \lceil n^{3/5} \rceil$, in order to show that larger $n_c$ will lead to more FPs. Generally speaking, we recommend to choose the $n_c$ rate between $n^{1/2}$ to $n^{3/4}$.

We conclude that in order to achieve the model consistency property, a small $n_c$ rate should be chosen as long as the size of the construction sample is large enough to provide accurate estimation. Despite the above comparison, the optimal $n_c$ rates may change when the settings are different.

6 Data Analysis

6.1 Eye Disease Gene Expression Dataset

We now illustrate one application of the proposed method via the dataset reported by Scheetz et al. (2006). In this dataset, for harvesting of tissue from the eyes and subsequent microarray analysis, 120 12-week-old male rats were selected. The microarrays used to analyze the RNA from the eyes of these animals contain more than 31,042...
Figure 3: CV($n_c$) Algorithm. False positives and negatives for different settings with different methods. The top row is linear regression results, and the bottom is logistic regression. The two panels on the left are for Lasso cases, the middle ones are SCAD, and the right ones are MCP. In each figure, the positive and negative parts are for false positives and negatives, respectively. Here, “——” is for 10-fold CV, “— —” for $n_c = \lceil n^{1/2} \rceil$, “·-” for $n_c = \lceil n^{7/12} \rceil$, “-·” for $n_c = \lceil n^{2/3} \rceil$, “—-” for $n_c = \lceil n^{3/4} \rceil$ and “—-” for $n_c = \lceil n^{4/5} \rceil$. In particular, in the top row, “-·” is for $n_c = \lceil n^{2/3} \rceil$; while in the bottom row, “—-” is for $n_c = \lceil n^{3/4} \rceil$. 

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Figure 4: CCV Algorithm. False positives and negatives for different settings with different methods. The top row is linear regression results, and the bottom is logistic regression. The panels on the left are for Lasso cases, the middle ones are SCAD, and the right ones are MCP. In each figure, the positive and negative parts are for false positives and negatives, respectively. Here, “——” is for 10-fold CV, “—” for $n_c = \lceil n^{1/2} \rceil$, “…” for $n_c = \lfloor n^{7/12} \rfloor$, “…” for $n_c = \lceil n^{2/3} \rceil$ and “— —” for $n_c = \lfloor n^{3/4} \rfloor$. In particular, in the top row, “— —” is for $n_c = \lceil n^{1/2} \rceil$; while in the bottom row, “…” is for $n_c = \lceil n^{2/3} \rceil$. 

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Table 4: Eye Disease Gene Expression Dataset. For CV($n_v$) and CCV, we have $n_c = \lceil n^{2/3} \rceil$ and $n_c = \lceil n^{1/2} \rceil$, respectively.

<table>
<thead>
<tr>
<th>penalty</th>
<th>CV($n_v$)</th>
<th>CCV</th>
<th>K-fold CV</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>size</td>
<td>PE</td>
<td>size</td>
</tr>
<tr>
<td>Lasso</td>
<td>24.95(12.81)</td>
<td>0.01(0.00)</td>
<td>2.45(0.68)</td>
</tr>
<tr>
<td>SCAD</td>
<td>20.20(5.35)</td>
<td>0.01(0.00)</td>
<td>2.34(0.67)</td>
</tr>
<tr>
<td>MCP</td>
<td>4.20(0.77)</td>
<td>0.01(0.00)</td>
<td>2.55(0.89)</td>
</tr>
</tbody>
</table>

different probe sets (Affymetric GeneChip Rat Genome 230 2.0 Array). The intensity values were normalized using the robust multichip averaging method (Irizarry et al., 2003) to obtain summary expression values for each probe set. Gene expression levels were analyzed on a logarithmic scale.

Following Huang et al. (2010) and Fan et al. (2011), we are interested in finding the genes that are related to the TRIM32 gene, which was recently found to cause Bardet-Biedl syndrome (Chiang et al., 2006) and is a genetically heterogeneous disease of multiple organ systems, including the retina. Although more than 30,000 probe sets are represented on the Rat Genome 230 2.0 Array, many of these are not expressed in the eye tissue. We focused only on the 18,975 probes that are expressed in the eye tissue.

We model this problem as a linear regression problem. We randomly draw without replacement 100 out of 120 observations from the sample, using them as training data, and use the remaining sub-sample of size 20 as the test data. We repeat this procedure 100 times with the results reported in Table 4 in the form of mean (standard deviation). For each split, we use glmnet and ncvreg to compute the Lasso and SCAD/MCP solution paths, respectively; and compared our proposed CV($n_v$) and CCV with the 10-fold CV, which is the default tuning parameter selection method in glmnet and ncvreg. For CV($n_v$) and CCV, we set $n_c = \lceil n^{2/3} \rceil = 22$ and $n_c = \lceil n^{1/2} \rceil = 10$, respectively.

For Lasso, compared with around 50 variables in K-fold CV, CCV selects around 2.5 variables on average to achieve the same prediction error. For SCAD and MCP, compared with 30 and 10 in K-fold CV, much smaller models are selected by CCV with the same prediction error. However, CV($n_v$) does not improve much in this case. We conjecture the possible reason is that the sample size is too small, and the size of the construction dataset is even smaller, which makes the algorithm unstable.

6.2 The Leukemia Dataset

We consider the leukemia dataset previously analyzed in Golub et al. (1999). There are $p = 7129$ genes and $n = 72$ samples coming from two classes: 47 in class ALL (acute lymphocytic leukemia) and 25 in class acute myelogenous leukemia (AML). To study the performance of the proposed methods, we randomly draw without replacement 100 times. Each time 12 out of 72 observations from the sample are selected as the test data, and the rest are the training data.

We model this problem as a logistic regression problem, and use glmnet and ncvreg to compute the Lasso and SCAD/MCP solution paths, respectively; and compare the proposed CV($n_v$) and CCV procedures with the 10-fold CV.
Table 5: The Leukemia Dataset. For CV($n_v$) and CCV, we have $n_c = \lceil n^{3/4}\rceil$ and $n_c = \lceil n^{2/3}\rceil$, respectively.

<table>
<thead>
<tr>
<th>penalty</th>
<th>CV($n_v$) size</th>
<th>CE(%)</th>
<th>CCV size</th>
<th>CE</th>
<th>K-fold CV size</th>
<th>CE(%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lasso</td>
<td>20.17(3.66)</td>
<td>6.17(3.57)</td>
<td>8.72(1.61)</td>
<td>5.17(8.92)</td>
<td>21.33(3.54)</td>
<td>5.00(5.67)</td>
</tr>
<tr>
<td>SCAD</td>
<td>15.80(0.84)</td>
<td>3.33(4.58)</td>
<td>5.90(1.58)</td>
<td>6.67(4.92)</td>
<td>17.60(3.20)</td>
<td>7.50(5.58)</td>
</tr>
<tr>
<td>MCP</td>
<td>5.20(2.59)</td>
<td>1.67(3.75)</td>
<td>4.65(1.56)</td>
<td>5.83(5.42)</td>
<td>5.25(1.33)</td>
<td>7.08(8.17)</td>
</tr>
</tbody>
</table>

In Table 5 we notice CCV has similar behavior for different types of penalty, especially for Lasso and SCAD. We use the classification error instead of prediction error in this example. In this case, CCV outperforms the 10-fold CV in terms of both parsimoniousness and accuracy of classification. Similarly, CV($n_v$) does not improve much from K-fold CV. Note that the sample size is even smaller than the previous real data example.

7 Discussion

In this paper we studied the theoretical properties and numerical behavior of different types of cross-validation methods applied to the tuning parameter selection problem in high-dimensional penalized generalized linear models. Both convex and folded-concave penalties are in the scope of this paper. For the commonly used cross-validation in high-dimensional settings, we investigated several possible reasons of over-selection. By putting K-fold CV into the larger framework of CV($n_v$), we show that the shrinkage caused by the penalty is not always the reason for over-selection with an appropriate choice of $n_v$. In addition, we proposed the Consistent Cross-Validation (CCV), which was shown to be consistent in very general settings.

One interesting future work is the theoretical behavior of CV($n_v$) in the penalized generalized linear model using convex and folded-concave penalties. This may require advanced techniques of the limiting distribution of extreme order statistics. There could also be an extension of the CCV to accommodate, among others, semiparametric models for survival data. Emphasis will be given to the Cox proportional hazards model, for which the penalized partial likelihood will be studied, and for the accelerated failure time model [Kalbfleisch and Prentice, 2002; Tsiatis, 1990; Ying, 1993], for which the $L_1$-type loss under different penalties will be studied. In addition, we are interested in selecting the concavity parameter $\gamma$ in folded-concave penalties.

8 Appendix

8.1 Proof of Lemma 1

Proof. Without loss of generality, we assume $\ell = k - 1$, and denote $T_k$ and $T_\ell$ as $T_1$ and $T_2$, respectively. Since in this problem, $k$ is fixed while $p$ diverges, this is an extreme order statistics problem [David and Nagaraja, 2003]. From Leadbetter et al. (1983)
and Pakshirajan and Hebbar (1977), there exists \(m_p^*\) satisfying

\[
\frac{1}{n} \sum_{i=1}^{p} \exp \left( a_p^*(m_i - m_p^*) - \frac{1}{2} (m_i - m_p^*)^2 \right) \rightarrow 1, \quad p \rightarrow \infty,
\]

where \(a_p^* = a_p - \log \log p / 2a_p\), \(a_p = (2 \log p)^{1/2}\), and also denote

\[
b_p = (2 \log p)^{1/2} - (1/2)(2 \log p)^{-1/2} (\log \log p + \log 4\pi).
\]

The limiting distribution of \(a_p(T_2 - b_p - m_p^*)\) is the Gumbel distribution, i.e.,

\[
P\{a_p(T_2 - b_p - m_p^*) \leq x\} \rightarrow \exp(-e^{-x}), \quad p \rightarrow \infty;
\]

and the joint limiting density of \((W_1, W_2) \equiv (a_p(T_1 - b_p - m_p^*), a_p(T_2 - b_p - m_p^*))\) is as follows.

\[
g_{W_1, W_2}(w_1, w_2) = g(w_1)g(w_2) / G(w_2), \quad w_1 < w_2,
\]

where \(g(\cdot)\) and \(G(\cdot)\) are the density and cumulative distribution functions of the Gumbel distribution, respectively. Thus, \(g_{W_1, W_2}(w_1, w_2) = e^{-w_2} g(w_1)\). Then we have,

\[
P\{kT_1^2 > (k-1)T_2^2\} = P\left\{W_1^2 > \frac{k-1}{k} W_2^2 - \frac{a_p b_p}{k}\right\}.
\]

Notice \(a_p b_p \rightarrow \infty\), as \(p \rightarrow \infty\), then

\[
\lim_{p} P\{kT_1^2 > (k-1)T_2^2\} = 1.
\]

---

8.2 Concentration Inequality

There are numerous concentration inequalities – to bound probabilities of deviations of a random variable from its mean or median. What we need here is a certain type of concentration inequality on a function, whereof the domain is a product space. To cater this purpose, Azuma’s inequality ([Azuma, 1967] [Hoeffding, 1963]) and McDiarmid’s inequality ([McDiarmid, 1989]), to name a few, are available.

Here we list the specific inequality we use in the sequel, which is provided in Lalley [2013] and adapted according to this paper. It helps us to develop the asymptotic theory where \(N\) – the size of the candidate models – is allowed to diverge with the sample size.

**Lemma 2.** (Gaussian concentration) Let \(\gamma\) be the standard Gaussian probability measure on \(\mathbb{R}^n\) (that is, the distribution of a \(\mathcal{N}(0, I)\) random vector), and let \(F : \mathbb{R}^n \rightarrow \mathbb{R}\) be Lipschitz in each variable separately relative to the Euclidean metric, with Lipschitz constant \(c\). Then for every \(t > 0\),

\[
\gamma\{|F - E\gamma F| \geq t\} \leq 2 \exp \left(-\frac{t^2}{c^2 \pi^2}\right).
\]
8.3 Proof of Theorem 1

Proof. Since in this theorem we consider averaging criterion values for each model, we have

\[ \hat{\Gamma}_\alpha = \frac{1}{rn_v} \sum_{s \in S} \left\| y_s - X_{s,\alpha} \hat{\beta}_{s',\alpha} \right\|^2 \]

\[ = \frac{1}{rn_v} \sum_{s \in S} \left\| y_s - X_{s,\alpha} \tilde{\beta}_{s',\alpha} \right\|^2 + \frac{1}{rn_v} \sum_{s \in S} \left\| X_{s,\alpha} \hat{\beta}_{s',\alpha} - X_{s,\alpha} \tilde{\beta}_{s',\alpha} \right\|^2 \]

\[ + \frac{2}{rn_v} \sum_{s \in S} (y_s - X_{s,\alpha} \tilde{\beta}_{s',\alpha})' (X_{s,\alpha} \hat{\beta}_{s',\alpha} - X_{s,\alpha} \tilde{\beta}_{s',\alpha}) \]

\( \triangleq \hat{\Gamma}_\alpha + \hat{\Gamma}_a + \hat{\Gamma}_a3. \)

From Theorem 1 of Shao (1993),

\[ \hat{\Gamma}_\alpha = \Delta_\alpha + \frac{1}{n} \varepsilon' \varepsilon + \frac{1}{n_c} d_\alpha \sigma^2 - \frac{1}{n} \varepsilon' P_\alpha \varepsilon + o \left( \frac{1}{n_c} \right), \]  

(8)

where \( \Delta_{\alpha,n} \equiv (1/n) \beta' X' (I_n - P_\alpha) X \beta, \) and we omit \( n \) in the subscript of \( \Delta. \)

Define \( \Sigma_{s,\alpha} = X_{s,\alpha}' X_{s,\alpha} \) and \( \Sigma_{s',\alpha} = X_{s',\alpha}' X_{s',\alpha}, \) and notice that

\[ \tilde{\beta}_{s',\alpha} = \Sigma_{s',\alpha}^{-1} X_{s',\alpha}' y_s \]

and \( \hat{\beta}_{s',\alpha} \) is the solution to

\[ \frac{1}{n} \Sigma_{s',\alpha}^{-1} \left( X_{s',\alpha}' \tilde{\beta}_{s',\alpha} - X_{s,\alpha} \hat{\beta}_{s',\alpha} \right) + \lambda_\alpha \text{sgn}(\tilde{\beta}_{s',\alpha}) = 0, \]

(10)

respectively. For any vector \( v \in \mathbb{R}^m, \text{sgn}(v) = (\text{sgn}(v_1), \cdots, \text{sgn}(v_m))'. \) From (9) and (10), we have

\[ \hat{\beta}_{s',\alpha} = \hat{\beta}_{s',\alpha} - n_c \lambda_\alpha \Sigma_{s',\alpha}^{-1} \text{sgn}(\tilde{\beta}_{s',\alpha}). \]

Then

\[ \hat{\Gamma}_\alpha = \frac{n_c^2}{rn_v} \sum_{s \in S} \lambda_\alpha^2 (\text{sgn}(\tilde{\beta}_{s',\alpha}))' \Sigma_{s',\alpha}^{-1} \Sigma_{s,\alpha} \Sigma_{s',\alpha}^{-1} \text{sgn}(\tilde{\beta}_{s',\alpha}). \]

(11)

Additionally, with Condition 3

\[ \hat{\Gamma}_\alpha = o(1) \hat{\Gamma}_a2. \]

(12)

Then, combining Condition 3, (8), (11) and (12), we have,

\[ \hat{\Gamma}_\alpha = \Delta_\alpha + \frac{1}{n} \varepsilon' \varepsilon + \frac{1}{n_c} d_\alpha \sigma^2 - \frac{1}{n} \varepsilon' P_\alpha \varepsilon + o \left( \frac{1}{n_c} \right) + d_\alpha \lambda_\alpha^2 (1 + o(1)). \]

(13)

Recall Wilks’ Theorem and the fact that in linear regression, \( E(\ell(\beta)) = (1/2) \beta' X' X \beta. \) Then for \( \alpha \in A \setminus A_c, \) we have \( \lim_n \Delta_{\alpha,n} > 0; \) otherwise \( \Delta_{\alpha,n} = 0. \) Moreover, from KKT
conditions, \( \lambda_\alpha \) is the maximum of \( (1/n_c) |x_{s',j}^c (y_{s'} - \mathbf{X}_{s',\alpha} \hat{\mathbf{\beta}}_{s',\alpha}) |, \ j \in \{1, \cdots, p\} \setminus \alpha \), i.e., the maximum order statistic of \( p - d_\alpha \) random variables. Note that
\[
\frac{1}{n_c} |x_{s',j}^c (y_{s'} - \mathbf{X}_{s',\alpha} \hat{\mathbf{\beta}}_{s',\alpha}) | = \left| \frac{1}{n_c} \sum_i r_{s',ij} (\mathbf{\beta}_i - \hat{\mathbf{\beta}}_i) + \frac{1}{n_c} x_{s',j}^c \varepsilon_{s'} \right|. \tag{14}
\]

Hence, \( \forall \alpha \in \mathbf{A} \setminus \mathbf{A}_c \),
\[
\Delta_\alpha + \frac{1}{n_c} d_\alpha \sigma^2 + d_\alpha \lambda_\alpha^2 - (\Delta_\alpha_1 + \frac{1}{n_c} d_\alpha \sigma^2 + d_\alpha \lambda_\alpha^2) > \beta_\alpha^2/2. \tag{15}
\]

In addition, we exploit Lemma 2 with \( F = \max_{\alpha \in \mathbf{A} \setminus \mathbf{A}_c} (1/n) (\varepsilon^T \mathbf{P}_\alpha \varepsilon - \varepsilon^T \mathbf{P}_\alpha \varepsilon) \), which is a function of independent \( \varepsilon \). First, we will prove \( F \) is Lipschitz with constant \( c \equiv 2\sqrt{d_\alpha/n} \) with probability tending to 1. Denote by \( \Omega_L(c) \) as this event. Then, we will use Gaussian concentration conditional on the event \( \Omega_L(c) \).

Notice
\[
|F(\varepsilon) - F(\varepsilon')| = \sup_\omega |\partial F(\varepsilon(\omega))/\partial \varepsilon(\omega)||d\varepsilon - \varepsilon' || d\varepsilon - \varepsilon' <= 2\sqrt{d_\alpha/n} \sup_\omega |\varepsilon_i(\omega)|/n \cdot ||d\varepsilon - \varepsilon' ||.
\]

The second inequality above holds by the fact that both \( \mathbf{P}_\alpha \) and \( \mathbf{P}_\alpha \) are projection matrices and \( \alpha \subset \alpha^c \) due to the path algorithm. We have
\[
\Omega_L(c) \supseteq \{ \omega : \sup_{1 \leq i \leq n} |\varepsilon_i(\omega)| \leq \sqrt{n} \}. \tag{16}
\]

Since \( \varepsilon_i \sim N(0,1) \), we have \( P(\varepsilon_i \geq t) \leq \frac{\exp(-(t^2/2)\sqrt{2\pi} \cdot t^2/2\pi} \) for \( t > 0 \). Using union bound,
\[
P(\Omega_L(c)) \geq 1 - \frac{2\sqrt{n} \exp(-n/2)}{\sqrt{2\pi}} = p_1 \to 1.
\]

Then from Condition 1 we have \( \forall \eta > 0 \),
\[
NP \{ |F - EF| > \eta \} \leq N(1 - p_1) + 2p_1 \exp(\log N - 2n\eta^2/d_\alpha) \to 0. \tag{17}
\]

Combining (15) and (16), also noticing that \( EF = d_\alpha \sigma^2/n \), we have
\[
P \left\{ \exists \alpha \in \mathbf{A} \setminus \mathbf{A}_c, \hat{\Gamma}_{\alpha_1} > \hat{\Gamma}_\alpha \right\} \to 0. \tag{18}
\]

i.e., the selected model will fall into the correct group with probability tending to 1.

For the candidate models in the correct category, we have the following discussion. Notice, for \( j, k \in \{1, \cdots, p\} \setminus \alpha, j \neq k \), \( \text{Corr}(x_{s',j}^c x_{s',k}^c, \varepsilon_{s'}^c) = r_{s',jk} \). By the fact that \( 1/n_c |\sum_i \rho_{s',ij} (\mathbf{\beta}_i - \hat{\mathbf{\beta}}_i) | = O(1) \), from Lemma 1 and using similar techniques as Proposition 1. \( \forall s \in \mathcal{S}, \mu \in [0,1], \hat{\Gamma}_{\alpha_2} \) is the dominating term in \( \hat{\Gamma}_\alpha \). Furthermore, for any \( \alpha \in \mathbf{A}_c \), but \( \alpha \neq \alpha_1 \),
\[
n_c \left( \frac{1}{n_c} d_\alpha \sigma^2 + d_\alpha \lambda_\alpha^2 - \frac{1}{n_c} d_\alpha \sigma^2 - d_\alpha \lambda_\alpha^2 \right) > 0.
\]

Similarly, applying Gaussian concentration with \( c \equiv 2\sqrt{(d_{\max} - d_\alpha)/n} \) and \( F = \max_{\alpha \in \mathbf{A}_c \setminus \{\alpha_1\}} (1/n) \varepsilon^T (\mathbf{P}_\alpha - \mathbf{P}_{\alpha_1}) \varepsilon \), we have
\[
P \left\{ \exists \alpha \in \mathbf{A}_c \setminus \{\alpha_1\}, \hat{\Gamma}_{\alpha_1} > \hat{\Gamma}_\alpha \right\} \to 0. \tag{19}
\]

Combining (17) and (19), the selection is consistent. \( \Box \)
8.4 Cross-Validation For GLM with Fixed Dimension Setting

Lemma 3. With \( p < n \), let \( \hat{\beta} \) be the MLE of a GLM. Assume the separable penalty function \( p(\cdot) \) is in the form of (2), and assume Conditions [2] - [7] hold. Furthermore, assume \( n_c \to \infty \) and \( n_c/n \to 0 \) as \( n \to \infty \), and the size of the splits \( r \) satisfies

\[
r^{-1}n_c^{-2}n^2 \to 0.
\]

Then, Monte Carlo Cross-Validation(\( n_v \)) is consistent.

Proof. Due to the properties of GLM models with canonical parameter, we have

\[
E(y_i|x_i) = \hat{b}(x_i', \beta), \quad \sigma_i^2 = a(\phi)\tilde{b}(x_i', \beta), \quad i = 1, \cdots, n,
\]

and define \( \sigma^2 = (1/n) \sum_{i=1}^n \sigma_i^2 \). The target is to select the model that minimizes the loss

\[
\hat{\Gamma}_\alpha = \frac{1}{rn_v} \sum_{s \in R} \left[ -y'_s(X_{s,\alpha}\tilde{\beta}_{s',\alpha}) + 1'b(X_{s,\alpha}\tilde{\beta}_{s',\alpha}) \right], \tag{19}
\]

where \( R \) represents the collection of validation sets in different splits.

Denote \( E_R \) and \( V_R \) as the expectation and variance with respect to the random selection of \( R \). By using the equality

\[
E_R \left( \frac{1}{r} \sum_{s \in R} a_s \right) = \left( \frac{n}{n_v} \right)^{-1} \sum_{s \in R} a_s,
\]

rewriting (19), and denoting \( \ell_s(\beta) = y'_s(X_s, \beta) - 1'b(X_s, \beta) \) and \( \ell_n(\tilde{\beta}_\alpha) = y'(X_s, \tilde{\beta}_\alpha) - 1'b(X_s, \tilde{\beta}_\alpha) \), we have

\[
E_R(\hat{\Gamma}_\alpha) = E_R \left( \frac{1}{rn_v} \sum_{s \in R} -\ell_s(\beta) \right) + E_R \left\{ \frac{1}{rn_v} \sum_{s \in R} \left[ \ell_s(\beta) - \left( y'_s(X_s, \tilde{\beta}_\alpha) - 1'b(X_{s,\alpha}\tilde{\beta}_{s',\alpha}) \right) \right] \right\} + E_R \left\{ \frac{1}{rn_v} \sum_{s \in R} \left[ \left( y'_s(X_s, \tilde{\beta}_\alpha) - 1'b(X_s, \tilde{\beta}_\alpha) \right) - \left( y'_s(X_{s,\alpha}\tilde{\beta}_{s',\alpha}) - 1'b(X_{s,\alpha}\tilde{\beta}_{s',\alpha}) \right) \right] \right\} = -\frac{1}{n} \ell_n(\beta) + \frac{1}{n} \left( \ell_n(\beta) - \ell_n(\tilde{\beta}_\alpha) \right) + \left( \frac{n}{n_v} \right)^{-1} \sum_{s \in R} \frac{1}{n_v} \left[ y'_s(X_s, \tilde{\beta}_\alpha) - X_{s,\alpha}\tilde{\beta}_{s',\alpha} \right] - 1' \left( b(X_s, \tilde{\beta}_\alpha) - b(X_{s,\alpha}\tilde{\beta}_{s',\alpha}) \right) \]

\[
\triangle - \frac{1}{n} \ell_n(\beta) + A_{\alpha 1} + \left( \frac{n}{n_v} \right)^{-1} \sum_{s \in R} A_{\alpha 2, s},
\]

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Notice that for different $\alpha$, $(1/n)\ell_n(\beta)$ stays the same, so we discuss $A_{a1}$ and $A_{a2,s}$ as follows.

From Wilks’ theorem, it is known that, if $\alpha \in \mathcal{A} \setminus \mathcal{A}_c$, as $n \to \infty$, we have $A_{a1} \xrightarrow{D} (1/2)\chi^2(k_\alpha)$, where $k_\alpha = d_0 - d_{a0}$, $d_{a0} = \#\{j : \beta_j \in \alpha \cap \alpha_0\}$, i.e., $k_\alpha$ is the number of false negatives. This means $E(A_{a1}) = k_\alpha$. Otherwise, $E(A_{a1}) = O(1/n)$.

Note that for any $s$,

$$1'\left(b(X_{s,a},\hat{\beta}_a) - b(X_{s,a},\hat{\beta}_{s,\alpha})\right) = b'(X_{s,a},\hat{\beta}_a)X_{s,a}(\hat{\beta}_a - \hat{\beta}_{s,\alpha})$$

$$- \frac{1}{2}(\hat{\beta}_a - \hat{\beta}_{s,\alpha})'X_{s,a}b'(X_{s,a},\hat{\beta}_a)X_{s,a}(\hat{\beta}_a - \hat{\beta}_{s,\alpha}) + o(1).$$

Define $u_{s'}(\gamma) = (1/n_c)X_{s',a}'(y_{s'} - b(X_{s',a},\gamma))$, then $\hat{\beta}_{s,\alpha}$ is the solution to $u_{s'}(\gamma) = 0$. By Taylor expansion, we get

$$\hat{\beta}_a - \hat{\beta}_{s,\alpha} = \left(\hat{u}_{s'}(\hat{\beta}_a)\right)^{-1}u_{s'}(\hat{\beta}_a)(1 + o(1)),$$

where $\hat{u}_{s'}(\hat{\beta}_a) = -(1/n_c)X_{s',a}'b(X_{s',a},\hat{\beta}_a)X_{s',a}$.

Define $D_{s,a} = b^{-1/2}(X_{s,a},\hat{\beta}_a)X_{s,a}$, then

$$A_{a2,s} = \frac{1}{n_v}\left(y_s - b(X_{s,a},\hat{\beta}_a)\right)'X_{s,a}(\hat{\beta}_a - \hat{\beta}_{s,\alpha})$$

$$+ \frac{1}{2n_v}(\hat{\beta}_a - \hat{\beta}_{s,\alpha})'X_{s,a}b'(X_{s,a},\hat{\beta}_a)X_{s,a}(\hat{\beta}_a - \hat{\beta}_{s,\alpha}) + o\left(\frac{1}{n_v}\right)$$

$$= \frac{1}{n_v}\left(y_s - b(X_{s,a},\hat{\beta}_a)\right)'X_{s,a}\left(\hat{u}_{s'}(\hat{\beta}_a)\right)^{-1}u_{s'}(\hat{\beta}_a) + o\left(\frac{1}{n_v}\right)$$

$$+ \frac{1}{2n_v}\left(y_{s'} - b(X_{s',a},\hat{\beta}_a)\right)'\left(b(X_{s',a},\hat{\beta}_a)^{-1/2}\right)D_{s,a}\left(D_{s,a}'D_{s,a}\right)^{-1}$$

$$\times \left(X_{s,a}b(X_{s,a},\hat{\beta}_a)X_{s,a}\right)\left(X_{s',a}b(X_{s',a},\hat{\beta}_a)X_{s',a}\right)^{-1}$$

$$\times D_{s,a}'\left(b(X_{s',a},\hat{\beta}_a)^{-1/2}\right)\left(y_{s'} - b(X_{s',a},\hat{\beta}_a)\right)(1 + o(1))$$

$$\hat{\triangle}B_a + C_a.$$

By plugging in the expansion form of $\hat{u}_{s'}(\cdot)$ and $u_{s'}(\cdot)$,

$$B_a = \frac{1}{n_v}\left(y_s - b(X_{s,a},\hat{\beta}_a)\right)'X_{s,a}\left(X_{s',a}b(X_{s',a},\hat{\beta}_a)X_{s',a}\right)^{-1}$$

$$\times X_{s',a}'\left(y_{s'} - b(X_{s',a},\hat{\beta}_a)\right)(1 + o(1)).$$

Considering the independent structure of different samples, Conditions 3 and 5, we have

$$E(B_a) = 0, \quad V(B_a) = \frac{d_{a0}a(\phi)}{\sqrt{n_vn_c}}(1 + o(1)). \quad (20)$$
And for $C_\alpha$ we have,

$$C_\alpha = \frac{1}{2n_c} \left( y_s - \bar{b}(X_{s,c} \tilde{\beta}_\alpha) \right)' \left( \bar{b}(X_{s,c} \tilde{\beta}_\alpha)^{-1/2} \right) D_{s,\alpha} \left( D'_{s,\alpha} D_{s,\alpha} \right)^{-1} D'_{s,\alpha} \times \left( \bar{b}(X_{s,c} \tilde{\beta}_\alpha)^{-1/2} \right) \left( y_s - \bar{b}(X_{s,c} \tilde{\beta}_\alpha) \right) \left( 1 + o(1) \right).$$

Thus, the desirable projection matrix shows up, and after taking expectation we have,

$$E(A_{\alpha,2,s}) = \frac{d_\alpha a(\phi)}{n_c} + o_p \left( \frac{1}{n_c} \right).$$

If $\alpha \in A \setminus A_c$,

$$\hat{\Gamma}_\alpha - \hat{\Gamma}_\alpha = \frac{1}{n} \left( \ell_n(\tilde{\beta}_\alpha) - \ell_n(\tilde{\beta}_\alpha) \right) + O \left( \frac{1}{n_c} \right).$$

From the similar techniques used in the proof of Theorem 1 by exploiting Gaussian concentration, $\forall \varepsilon > 0$, we have

$$NP \left\{ n_c \left| \max_{\alpha \in A \setminus A_c} \left| \frac{1}{n} \left( \ell_n(\tilde{\beta}_\alpha) - \ell_n(\tilde{\beta}_\alpha) \right) \right| - E \left( \max_{\alpha \in A \setminus A_c} \left| \frac{1}{n} \left( \ell_n(\tilde{\beta}_\alpha) - \ell_n(\tilde{\beta}_\alpha) \right) \right| \right| > \varepsilon \right\} \rightarrow 0.$$

The parallel result for $\alpha \in A_c$ but $\alpha \neq \alpha_*$ holds similarly, i.e., as $n \rightarrow \infty$,

$$P \{ \hat{\alpha} = \alpha_* \} \rightarrow 1.$$

References


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