Multiclass classification by sparse multinomial logistic regression

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Abstract

In this paper we consider high-dimensional multiclass classification by sparse multinomial logistic regression. We propose a feature selection procedure based on penalized maximum likelihood with a complexity penalty on the model size and derive the nonasymptotic bounds for misclassification excess risk of the resulting classifier. We establish also their tightness by deriving the corresponding minimax lower bounds. In particular, we show that there exist two regimes corresponding to small and large number of classes. The bounds can be reduced under the additional low noise condition. Implementation of any complexity penalty based procedure, however, requires a combinatorial search over all possible models. To find a feature selection procedure computationally feasible for high-dimensional data, we propose multinomial logistic group Lasso and Slope classifiers and show that they also achieve the optimal order in the minimax sense.

Keywords: Complexity penalty; convex relaxation; feature selection; high-dimensionality; minimaxity; misclassification excess risk; sparsity.
1 Introduction

Classification is one of the core problems in statistical learning and has been intensively studied in statistical and machine learning literature. Nevertheless, while the theory for binary classification is well developed (see, Devroy, Györfi and Lugosi, 1996; Vapnik, 2000; Boucheron, Bousquet and Lugosi, 2005 and references therein for a comprehensive review), its multiclass extensions are much less complete.

Consider a general $L$-class classification with a (high-dimensional) vector of features $X \in \mathcal{X} \subseteq \mathbb{R}^d$ and the outcome class label $Y \in \{1, \ldots, L\}$. We can model it as $Y|(X = x) \sim \text{Mult}(p_1(x), \ldots, p_L(x))$, where $p_l(x) = P(Y = l|X = x)$, $l = 1, \ldots, L$.

A classifier is a measurable function $\eta: \mathcal{X} \to \{1, \ldots, L\}$. The accuracy of a classifier $\eta$ is defined by a misclassification error $R(\eta) = P(Y \neq \eta(x))$. The optimal classifier that minimizes this error is the Bayes classifier $\eta^*(x) = \arg\max_{1 \leq l \leq L} p_l(x)$ with $R(\eta^*) = 1 - E_X \max_{1 \leq l \leq L} p_l(x)$.

The probabilities $p_l(x)$’s are, however, unknown and one should derive a classifier $\hat{\eta}(x)$ from the available data $D$: a random sample of $n$ independent observations $(X_1, Y_1), \ldots, (X_n, Y_n)$ from the joint distribution of $(X, Y)$. The corresponding (conditional) misclassification error of $\hat{\eta}$ is $R(\hat{\eta}) = P(Y \neq \hat{\eta}(x)|D)$ and the goodness of $\hat{\eta}$ w.r.t. $\eta^*$ is measured by the misclassification excess risk $E(\hat{\eta}, \eta^*) = ER(\hat{\eta}) - R(\eta^*)$. The goal is then to find a classifier $\hat{\eta}$ within given family with minimal $E(\hat{\eta}, \eta^*)$.

A crucial drawback of ERM is in minimization of 0-1 loss that makes it computationally infeasible. A typical remedy is to replace 0-1 loss by a related convex surrogate. The resulting solution approximates then the minimizer of the corresponding surrogate risk.

A first strategy in multiclass classification is to reduce it to a series of binary classifications. The probably two most well-known methods are One-vs-All (OvA), where each class is compared against all others, and One-vs-One (OvO), where all pairs of classes are compared to each other.

A more direct and appealing strategy is to extend binary classification approaches for multiclass case. Thus, a common approach to design a multiclass classifier $\hat{\eta}$ is based on empirical risk minimization (ERM), where minimization of a true misclassification error $R(\eta)$ is replaced by minimization of the corresponding empirical risk $\hat{R}_n(\eta) = \frac{1}{n} \sum_{i=1}^n I\{Y_i \neq \eta(x_i)\}$ over a given class of classifiers. For binary classification, tight risk bounds for ERM classifiers have been established in terms of VC-dimension, Rademacher complexity or covering numbers (see Devroy, Györfi and Lugosi, 1996; Vapnik, 2000; Boucheron, Bousquet and Lugosi, 2005 and references therein). Their extensions to multiclass case, however, are not straightforward. See Maximov and Reshetova (2016) for a comprehensive survey of the state-of-the-art results on the upper bounds for misclassification excess risk of multiclass ERM classifiers. A comparison of error bounds for ERM classifiers with those for OvA and OvO is given in Danieli et al. (2012).
or calibrated loss). Various calibrated losses for multiclass classification have been considered in the literature (e.g., Zhang, 2004b; Chen and Sun, 2006; Tewari and Bartlett, 2007; Ávila Pires, Szepesvári and Ghavamzadeh, 2013; Ávila Pires and Szepesvári, 2016).

An alternative approach to ERM is to estimate \( p_l(x) \)'s from the data by some \( \hat{p}_l(x) \)'s and to use a plug-in classifier of the form \( \hat{\eta}(x) = \arg \max_{1 \leq l \leq L} \hat{p}_l(x) \). A standard approach is to assume some (parametric or nonparametric) model for \( p_l(x) \). The most commonly used model is multinomial logistic regression, where it is assumed that
\[
p_l(x) = \frac{\exp(\beta_l^T x)}{\sum_{k=1}^{L} \exp(\beta_k^T x)}
\]
and \( \beta_l \in \mathbb{R}^d \), \( l = 1, \ldots, L \) are unknown vectors of regression coefficients. The corresponding Bayes classifier is, therefore, a linear classifier
\[
\eta^*(x) = \arg \max_{1 \leq l \leq L} p_l(x) = \arg \max_{1 \leq l \leq L} \beta_l^T x.
\]
One then estimates \( \beta_l \)'s from the data by the maximum likelihood estimators (MLE) \( \hat{\beta}_l \)'s and derives the plug-in (linear) classifier \( \hat{\eta}(x) = \arg \max_{1 \leq l \leq L} \hat{\beta}_l^T x \). Unlike ERM, the MLE \( \hat{\beta}_l \)'s though not available in the closed form, can be nevertheless obtained numerically by the fast iteratively reweighted least squares algorithm (McCullagh and Nelder, 1989, Section 2.5).

The general challenge modern statistics faces with is high-dimensionality of the data, where the number of features \( d \) is large and might be even larger than the sample size \( n \) (large \( d \) small \( n \) setups) that raises a severe “curse of dimensionality” problem. Reducing the dimensionality of a feature space by selecting a sparse subset of “significant” features becomes crucial.

For binary classification Devroy, Györfi and Lugosi (1996, Chapter 18) and Vapnik (2000, Chapter 4) considered model selection from a sequence of classifiers within a sequence of classes by penalized ERM with the structural penalty depending on the VC-dimension of a class. See also Boucheron, Bousquet and Lugosi (2005, Section 8) for related penalized ERM approaches and references therein. Abramovich and Grinshtein (2019) explored feature selection in high-dimensional logistic regression classification.

To the best of our knowledge, feature selection for multiclass classification has not yet been rigorously well-studied and the goal of this paper is to fill the gap. Thus, we propose a model/feature selection procedure based on penalized maximum likelihood with a certain complexity penalty on the model size. We establish the non-asymptotic upper bounds for misclassification excess risk of the resulting plug-in classifier which is also adaptive to the unknown sparsity and show their tightness by deriving the corresponding minimax lower bound over a set of sparse linear classifiers. In particular, we find that there exist two regimes. For \( L \leq 2 + \ln(d/d_0) \), where \( d_0 \) is the size of the true (unknown) model, the multiclass effect is not manifested and the minimax misclassification excess risk over the set of \( d_0 \)-sparse linear classifiers is of the order \( \sqrt{\frac{d_0 \ln \left( \frac{d_0}{d_0} \right)}{n}} \) regardless of \( L \). For larger \( L \), it increases as \( \sqrt{\frac{d_0 (L-1)}{n}} \) and does not depend on \( d \). We also show that these bounds can be improved under the additional low-noise assumption.

Any penalized maximum likelihood procedure that involves a complexity penalty requires, however, a combinatorial search over all possible models that makes its use computationally infeasible.
for large $d$. A common remedy is then to use a convex surrogate, where the original combinatorial minimization is replaced by a related convex program. In this paper we consider Slope convex relaxation which can be viewed as generalization of the celebrated Lasso and show that for the properly chosen tuning parameters, the resulting multinomial logistic group Slope multiclass classifier is also minimax rate-optimal.

The rest of the paper is organized as follows. In Section 2 we present sparse multinomial logistic regression model and propose a feature selection procedure. The bounds for misclassification excess risk of the resulting plug-in classifier are derived in Section 3. In Section 4 we introduce the additional low-noise assumption that allows one to improve the bounds. In Section 5 we develop group Slope convex relaxation techniques for multiclass classification with Lasso as its particular case, and establish the misclassification excess risk bounds for the resulting classifier. All the proofs are given in the Appendix.

2 Construction of a classifier

2.1 Multinomial logistic regression model

Consider $d$-dimensional $L$-class classification model that can be written in the following form:

$$Y|(X = x) \sim Mult(p_1(x), \ldots, p_L(x)),$$

where $X \in \mathbb{R}^d$ is a vector of features with a marginal probability distribution $P_X$ of bounded support $\mathcal{X} \subset \mathbb{R}^d$ and $\sum_{j=1}^L p_j(x) = 1$ for any $x \in \mathcal{X}$. By re-scaling we can assume without loss of generality that the Euclidean norm $|x|_2 \leq 1$ for all $x \in \mathcal{X}$.

Assume that all features $X_j$ are linearly independent and, therefore, the minimal eigenvalue $\lambda_{\min}(G)$ of the matrix $G = E(XX^t)$ is strictly positive.

We consider a multinomial logistic regression model, where it is assumed that

$$\ln \frac{p_l(x)}{p_L(x)} = \beta_l^t x, \quad l = 1, \ldots, L - 1,$$

and $\beta_l \in \mathbb{R}^d$ are the vectors of the (unknown) regression coefficients. Hence,

$$p_l(x) = \frac{\exp(\beta_l^t x)}{1 + \sum_{k=1}^{L-1} \exp(\beta_k^t x)}, \quad l = 1, \ldots, L - 1 \quad \text{and} \quad p_L(x) = \frac{1}{1 + \sum_{k=1}^{L-1} \exp(\beta_k^t x)},$$

or, in a somewhat more compact form,

$$p_l(x) = \frac{\exp(\beta_l^t x)}{\sum_{k=1}^{L} \exp(\beta_k^t x)}, \quad l = 1, \ldots, L$$

with $\beta_L = 0$. We set $\beta_l = \infty = (\infty, \ldots, \infty)$ and $\beta_l = -\infty = (-\infty, \ldots, -\infty)$ to include two degenerate cases $p_l(x) = 1$ and $p_l(x) = 0$ respectively.
The Bayes classifier is then a linear classifier \( \eta^*(x) = \arg \max_{1 \leq i \leq L} p_l(x) = \arg \max_{1 \leq i \leq L} \beta_i^t x \) with misclassification risk \( R(\eta^*) = 1 - E_X \max_{1 \leq i \leq L} p_l(x) \).

The choice of the last class as a reference class is, in fact, quite arbitrary. One can consider an equivalent model with any other reference class \( h \) instead: \( \ln \frac{p_l(x)}{p_h(x)} = \gamma_l x, \quad l \neq h \). Evidently, there is one-to-one transformation: \( \gamma_l = \beta_l - \beta_h \) and \( \beta_l = \gamma_l - \gamma_L \). Change of a reference class is, therefore, just a matter of reparametrization of the same model.

### 2.2 Penalized maximum likelihood estimation

To each possible value \( y \in \{1, \ldots, L\} \) of \( Y \) assign the indicator vector \( \xi \in \{0,1\}^L \) with \( \xi_l = 1 \{ y = l \} \), \( l = 1, \ldots, L \). Let \( B \in \mathbb{R}^{d \times L} \) be the matrix of the regression coefficients in (2) with the columns \( \beta_1, \ldots, \beta_L \) (recall that \( \beta_L = 0 \)) and let \( f_B(x,y) \) be the corresponding joint distribution of \( (X,Y) \), i.e., \( df_B(x,y) = \prod_{l=1}^L p_l(x)\xi_l \, dP_X(x) \), where \( p_l(x) = \frac{\exp(\beta_l^t x)}{\sum_{k=1}^L \exp(\beta_k^t x)} \). Given a random sample \( (X_1,Y_1), \ldots, (X_n,Y_n) \sim f_B(X,Y) \), the log-likelihood function is

\[
\ell(B) = \sum_{i=1}^n \left\{ X_i^t B \xi_i - \ln \sum_{l=1}^L \exp(\beta_l^t X_i) \right\},
\]

where \( \xi_i \) is the indicator vector corresponding to \( Y_i \), and one can find the maximum likelihood estimator (MLE) for \( B \).

The era of “Big Data” brought the challenge of dealing with situations, where the number of features \( d \) is very large and may be even larger than the sample size \( n \) (“large \( d \) small \( n \)” setups). Nevertheless, it is commonly assumed that the true underlying model is sparse and most of the features do not have a significant impact on classification. Reducing the dimensionality of a feature space by selecting a sparse subset of “significant” features is then crucial. Thus, Bickel and Levina (2004) and Fan and Fan (2008) showed that even for binary classification, high-dimensional classification without a proper feature selection might be as bad as just pure guessing.

For binary classification, where the regression matrix \( B \) reduces to a single vector \( \beta \in \mathbb{R}^d \), the sparsity is naturally measured by the \( l_0 \) (quasi)-norm \( |\beta|_0 \) – the number of non-zero entries of \( \beta \) (see, e.g., Abramovich and Grinshtein, 2019). For multiclass case one can think of several possible ways to extend the notion of sparsity. The most evident measure of sparsity is the number of non-zero rows of \( B \) that corresponds to the assumption that part of the features do not have any impact on classification at all and, therefore, have zero coefficients in (2) for all \( l \). It can be viewed as *global* sparsity. One can easily verify that such a measure is invariant under the choice of the reference class in (2).

In what follows we assume the following assumption:

**Assumption (A).** Assume that there exists \( 0 < \delta < 1/2 \) such that \( \delta < p_l(x) < 1 - \delta \) or, equivalently, \( |\beta_l^t x| < C_0 \) with \( C_0 = \ln \frac{1-\delta}{\delta} \) for all \( x \in X \) and all \( l = 1, \ldots, L \). In particular, for \( |x|_2 \leq 1 \), it is sufficient to assume the boundedness of \( \beta_l \)'s, i.e., \( |B|_{2,\infty} = \max_{1 \leq l \leq L} |\beta_l|_2 \leq C_0 \).
Assumption (A) prevents the variances $\text{Var}(\xi_l) = p_l(x)(1 - p_l(x))$ to be infinitely close to zero, where any MLE-based procedure may fail.

Let $\mathfrak{M}$ be the set of all $2^d$ possible models $M \subseteq \{1, \ldots, d\}$. In view of Assumption (A), for a given model $M$ define a set of matrices $\mathcal{B}_M = \{B \in \mathbb{R}^{d \times L} : B_L = 0, |B|_\infty \leq \frac{1-\delta}{\delta} \text{ and } B_j = 0 \text{ iff } j \not\in M\}$. Obviously, all matrices in $\mathcal{B}_M$ have the same number of non-zero rows which can be naturally defined as a model size $|M|$.

Under the model $M$, the MLE $\hat{B}_M$ of $B$ is then

$$\hat{B}_M = \arg \max_{\hat{B} \in \mathcal{B}_M} \left\{ \sum_{i=1}^n \left( X_i^T \hat{B} \xi_i - \ln \sum_{l=1}^L \exp(\hat{\beta}_l^T X_i) \right) \right\},$$

where $\hat{\beta}_l = \hat{B}_l$, $l = 1, \ldots L$ are the columns of $\hat{B}$.

We now select the model $\hat{M}$ by the penalized maximum likelihood model selection criterion of the form

$$\hat{M} = \arg \min_{M \in \mathfrak{M}} \left\{ \sum_{i=1}^n \left( \ln \left( \sum_{l=1}^L \exp(\hat{\beta}_l^T M_l x_i) \right) - X_i^T \hat{B}_M \xi_i \right) + Pen(|M|) \right\}$$

with the complexity penalty $Pen(\cdot)$ on the model size $|M|$.

Finally, for the selected model $\hat{M}$ the resulting plug-in classifier

$$\hat{\eta}_{\hat{M}}(x) = \arg \max_{1 \leq l \leq L} \hat{\beta}_l^T \hat{M}_l x$$

The proper choice of the complexity penalty $Pen(\cdot)$ in (5) is obviously the core of the proposed approach.

## 3 Misclassification excess risk bounds

We now derive the (non-asymptotic) upper bound for misclassification excess risk of the penalized maximum likelihood classifier (6) derived in Section 2 for a particular type of the complexity penalty and then show that such a choice is, in fact, optimal (in the minimax sense).

Denote the number of nonzero rows of a matrix $B$ by $r_B$. Let $\mathcal{C}_L(d_0) = \{\eta(x) = \text{arg max}_{1 \leq l \leq L} \beta_l^T x : B \in \mathbb{R}^{d \times L}, B_L = 0 \text{ and } r_B \leq d_0\}$ be the set of all $d_0$-sparse linear $L$-class classifiers. The sparsity parameter $d_0$ is assumed to be unknown and the goal is to construct classifiers adaptive to the unknown sparsity.

**Theorem 1.** Consider a $d_0$-sparse multinomial logistic regression model (1)-(2).

Let $\hat{M}$ be a model selected in (4)-(5) with the complexity penalty

$$Pen(|M|) = c_1 |M|(|L|-1) + c_2 |M| \ln \left( \frac{d e}{|M|} \right),$$

where the absolute constants $c_1, c_2 > 0$ are given in the proof of Theorem 3.
Then, under Assumption (A),

$$
\sup_{\eta^* \in C_{L}(d_0)} \mathcal{E}(\hat{\eta}^{\hat{M}}, \eta^*) \leq C_1(\delta, \lambda_{\min}(G)) \sqrt{\frac{d_0(L - 1) + d_0 \ln \left( \frac{d}{d_0} \right)}{n}}
$$

(8)

for some $C_1(\delta, \lambda_{\min}(G))$ depending on $\delta$ and $\lambda_{\min}(G)$, simultaneously for all $1 \leq d_0 \leq \min(d, n)$.

Theorem 1 is a particular case of a more general Theorem 3 given in the next Section 4.

The complexity penalty $\text{Pen}(|M|)$ in (7) contains two terms. The first one is proportional to $|M| (L - 1)$ – the overall number of estimated parameters in the model $M$ and is an AIC-type penalty. The second one is proportional to $|M| \ln \left( \frac{d}{|M|} \right) \sim \ln \left( \frac{d}{|M|} \right)$ – the log(number of all possible models of size $|M|$) and typically appears in model selection in various regression and classification setups (see, e.g. Birgé and Massart, 2001; Bunea, Tsybakov and Wegkamp, 2007; Abramovich and Grinshtein, 2010, 2016, 2019).

Theorem 2 below shows that for the agnostic model, where the Bayes risk $R(\eta^*) > 0$, the upper bound (8) for the misclassification excess risk established in Theorem 1 is essentially tight and up to a possibly different constant coincides with the corresponding minimax lower bound over $C_{L}(d_0)$:

**Theorem 2.** Consider a $d_0$-sparse agnostic multinomial logistic regression model (1)-(2), where $2 \leq d_0 \ln \left( \frac{d}{d_0} \right) \leq n$ and $d_0(L - 1) \leq n$. Then,

$$
\inf_{\tilde{\eta}} \sup_{\eta^* \in C_{L}(d_0), P_X} \mathcal{E}(\tilde{\eta}, \eta^*) \geq C_2 \sqrt{\frac{d_0(L - 1) + d_0 \ln \left( \frac{d}{d_0} \right)}{n}}
$$

for some $C_2 > 0$, where the infimum is taken over all classifiers $\tilde{\eta}$ based on the data $(X_i, Y_i)$, $i = 1, \ldots, n$.

The above bounds imply, in particular, that as $d$ and $L$ grow with $n$ and assuming that $\delta$ and $\lambda_{\min}(G)$ are bounded away from zero, there are two different regimes:

1. **Small number of classes:** $L \leq 2 + \ln \left( \frac{d}{d_0} \right)$.
   In this case, the complexity penalty (7) is $\text{Pen}(|M|) \sim c|M| \ln \left( \frac{d}{|M|} \right)$ does not depend on $L$. The resulting (rate-optimal) misclassification excess risk is of the order $\sqrt{\frac{d_0 \ln \left( \frac{d}{d_0} \right)}{n}}$ regardless of $L$ and the error in feature selection dominates in the overall excess risk. Multiclass classification for such a small number of classes is essentially not harder than binary (see the results of Abramovich and Grinshtein, 2019 for $L = 2$).

2. **Large number of classes:** $2 + \ln \left( \frac{d}{d_0} \right) < L \leq \frac{n}{d_0}$.
   In this regime, $\text{Pen}(|M|) \sim c|M|(L - 1)$ is an AIC type penalty (see above), the misclassification excess risk increases with $L$ as $\sqrt{\frac{d_0(L - 1)}{n}}$ regardless of $d$ and the main contribution to the overall error comes from estimating the large number ($d_0(L - 1)$) of parameters in the model.
For $L > \frac{n}{d_0}$ the number of parameters in the model becomes larger than the sample size and consistent classification is impossible.

In particular, without sparsity assumption, i.e. in the case $d_0 = d$, the misclassification excess risk is of the order $\sqrt{\frac{d(L-1)}{n}}$ for all $2 \leq L \leq \frac{n}{n}$.

Note that even if the considered multinomial logistic regression model is misspecified and the Bayes classifier $\eta^*$ is not linear, we still have the following risk decomposition

$$R(\hat{\eta}_M) - R(\eta^*) = (R(\hat{\eta}_M) - R(\eta^*_L)) + (R(\eta^*_L) - R(\eta^*)),$$

where $\eta^*_L = \arg\min_{\eta \in \mathcal{C}(d)} R(\eta)$ is the oracle (ideal) linear classifier. The above results can then be still applied to the first term in the RHS of (9) representing the estimation error, while the second term is an approximation error and measures the ability of linear classifiers to perform as good as $\eta^*$. Enriching the class of classifiers may improve the approximation error but will necessarily increase the estimation error in (9). In a way, it is similar to the variance/bias tradeoff in regression.

### 4 Improved bounds under low-noise condition

Intuitively, it is clear that misclassification error is particularly large when it is difficult to separate the class with the highest probability from others, i.e. at those $x \in \mathcal{X}$, where the largest probability $p_{(1)}(x)$ is close to the second largest $p_{(2)}(x)$ (see also Kesten and Morse, 1959).

Define the following multiclass extension of the low-noise (aka Tsybakov) condition (Mammen and Tsybakov, 1999; Tsybakov, 2004):

**Assumption (B).** Consider the multinomial logistic regression model (1)-(2) and assume that there exist $C > 0, \alpha \geq 0$ and $h^* > 0$ such that for all $0 < h \leq h^*$,

$$P(p_{(1)}(X) - p_{(2)}(X) \leq h) \leq Ch^\alpha$$

(see also Agarwal, 2013). Assumption (B) implies that with high probability (depending on the parameter $\alpha$) the most likely class is sufficiently distinguished from others. The two extreme cases $\alpha = 0$ and $\alpha = \infty$ correspond respectively to the case without any assumption on the noise considered in the previous sections and the noiseless case. A straightforward multiclass extension of Lemma 5 of Bartlett, Jordan and McAuliffe (2006) implies that (10) is equivalent to the condition that there exists $C_1(\alpha)$ such that for any classifier $\eta$,

$$P(\eta(X) \neq \eta^*(X)) \leq C_1(\alpha) \mathcal{E}(\eta, \eta^*)^\frac{\alpha}{\alpha+1}$$

We now show that under the additional low-noise condition (10), the bounds for the misclassification excess risks established in the previous Section 3 can be improved:
Theorem 3. Consider a $d_0$-sparse multinomial logistic regression model (1)-(2) and let $\hat{M}$ be a model selected in (5) with the complexity penalty (7).

Then, under Assumptions (A) and (B), there exists $C(\delta, \lambda_{\text{min}}(G))$ such that

$$\sup_{\eta^* \in \mathcal{C}(d_0)} \mathcal{E}(\eta^*_M, \eta^*) \leq C(\delta, \lambda_{\text{min}}(G)) \left( d_0(L-1) + d_0 \ln \left( \frac{d_0}{d_0} \right) \right)^{\frac{\alpha+1}{\alpha+2}}$$

for all $1 \leq d_0 \leq \min(d, n)$ and all $\alpha \geq 0$.

Thus, $\hat{\eta}_M$ is adaptive to both $d_0$ and $\alpha$. As we have mentioned, Theorem 1 is a particular case of Theorem 3 with $\alpha = 0$.

5 Multinomial logistic group Lasso and Slope

Despite strong theoretical results on penalized maximum likelihood classifiers with complexity penalties established in the previous sections, selecting the model $\hat{M}$ in (5) requires a combinatorial search over all possible models in $\mathcal{M}$ that makes it computationally infeasible when the number of features is large. A common approach to handle this problem is convex relaxation, where the original combinatorial minimization is replaced by a related convex surrogate. The most well-known examples include the celebrated Lasso, where the $l_0$-norm in the penalty is replaced by $l_1$-norm norm, and its recently developed more general variation Slope that uses a sorted $l_1$-type norm (Bogdan et al., 2015). Lasso and Slope estimators have been intensively studied in Gaussian regression (see, e.g., Bickel, Ritov and Tsybakov, 2009; Su and Candés, 2015; Bellec, Lecué and Tsybakov, 2018 among others), and their logistic modifications in logistic regression (van de Geer, 2008; Abramovich and Grinshtein, 2019; Alquier, Cottet and Lecué, 2019). Abramovich and Grinshtein (2019) investigated logistic Lasso and Slope classifiers for the binary case. In this section we consider multinomial logistic group Lasso and Slope classifiers and extend the corresponding results of Abramovich and Grinshtein (2019) for multiclass classification.

Recall that we consider a global sparsity, where the coefficient regression matrix $B$ has a subset of zero rows. To capture such type of sparsity we consider a multinomial logistic group Lasso and Slope classifiers defined as follows. For a given tuning parameter $\lambda > 0$, find

$$\hat{B}_{gL} = \arg \min_{\hat{B}} \left\{ \frac{1}{n} \sum_{i=1}^{n} \left( \ln \left( \sum_{l=1}^{L} \exp(\hat{\beta}_l^t X_i) \right) - X_i^t \hat{B} \xi_i \right) + \lambda \sum_{j=1}^{d} |\hat{B}|_j \right\}, \quad (12)$$

where $|\hat{B}|_j = |\hat{B}_{j,:}|_2$ is the $l_2$-norm of the $j$-th row of $\hat{B}$ and define the corresponding classifier $\hat{\eta}_{gL}(x) = \arg \max_{1 \leq l \leq L} \hat{\beta}_{gL,l} x$. An efficient algorithm for computing multinomial logistic group Lasso is given in Vincent and Hansen (2014).
Multinomial logistic group Slope is a more general variation of (12). Namely,

$$
\hat{B}_{gS} = \arg \min_B \left\{ \frac{1}{n} \sum_{i=1}^{n} \left( \ln \left( \sum_{l=1}^{L} \exp(\tilde{\beta}_l^t X_i) \right) - X_i^t \tilde{B} \xi_i \right) + \sum_{j=1}^{d} \lambda_j |\bar{B}|_{(j)} \right\},
$$

(13)

where the rows’ l2-norms $|\bar{B}|_{(1)} \geq \ldots \geq |\bar{B}|_{(d)}$ are the descendingly ordered and $\lambda_1 \geq \ldots \geq \lambda_d > 0$ are the tuning parameters, and set $\tilde{\eta}_{gS}(x) = \arg \max_{1 \leq l \leq L} \tilde{\beta}_{gS,l} x$. Multivariate logistic group Lasso (12) can be evidently viewed as a particular case of (13) with equal $\lambda_j$’s.

Note that unlike complexity penalties, the solution of (13) is identifiable without the additional constraint $\tilde{\beta}_L = 0$. Moreover, since the unconstrained log-likelihood (3) satisfies $\ell(\tilde{\beta}_1, \ldots, \tilde{\beta}_L) = \ell(\tilde{\beta}_1 - c, \ldots, \tilde{\beta}_L - c)$ for any vector $c \in \mathbb{R}^d$, the solution can be always improved by taking $\hat{c}_j = \arg \min_{c_j} \sum_{l=1}^{L} (\tilde{B}_{jl} - c_j)^2$, i.e. $\hat{c}_j = \tilde{B}_{j}$. Hence, $\hat{B}_{gS}$ necessarily satisfies the symmetric constraint $\sum_{l=1}^{L} \tilde{\beta}_{gS,l} = 0$ or, equivalently, $\hat{B}_{gS}1 = 0$.

Consider a general multinomial logistic group Slope classifier with $\lambda_j$’s depending possibly on $n$, $d$ and $L$. The following theorem provides an upper bound for its misclassification excess risk:

**Theorem 4.** Consider a $d_0$-sparse multinomial logistic regression (1)-(2).

Apply the multinomial logistic group Slope classifier (13) with $\lambda_j$’s satisfying

$$
\max_{1 \leq j \leq d} \sqrt{\frac{L + \ln(d/j)}{\lambda_j}} \leq C_1 \sqrt{n}
$$

(14)

with the constant $C_1$ derived in the proof.

Then, under Assumptions (A) and (B),

$$
\sup_{\eta^* \in \mathcal{C}_L(d_0)} \mathcal{E}(\tilde{\eta}_{gS}, \eta^*) \leq C(\delta) \left( \sum_{j=1}^{d_0} \frac{\lambda_j}{\sqrt{j}} \right)^{2(\alpha+1)/\alpha+2}
$$

for some constant $C(\delta)$ depending on $\delta$.

We now consider two specific choices of $\lambda_j$’s:

1. Equal $\lambda_j$ (multinomial logistic group Lasso).

Take

$$
\lambda = C_1 \sqrt{\frac{L + \ln d}{n}}
$$

(15)

to satisfy (14). Note that $\sum_{j=1}^{d_0} \frac{1}{\sqrt{j}} \leq 2\sqrt{d_0}$ that yields the following corollary of Theorem 4.

**Corollary 1.** Consider a $d_0$-sparse multinomial logistic regression (1)-(2). Apply the multinomial logistic group Lasso classifier (12) with $\lambda$ from (15).

Then, under Assumptions (A) and (B),

$$
\sup_{\eta^* \in \mathcal{C}_L(d_0)} \mathcal{E}(\tilde{\eta}_{gL}, \eta^*) \leq C(\delta) \left( \frac{d_0(L-1) + d_0 \ln(d)}{n} \right)^{\alpha+1/\alpha+2}
$$

for all $1 \leq d_0 \leq \min(d, n)$ and all $\alpha \geq 0$. 


Thus, the multinomial logistic group Lasso classifier \( \hat{\eta}_{gL} \) is of a minimax order for large number of classes (see Section 3), while for small \( L \) it is rate-optimal for sparse cases, where \( d_0 \ll d \), but only sub-optimal (up to an extra logarithmic loss) for dense cases, where \( d_0 \sim d \). We conjecture that similar to the results of Bellec, Lecuée and Tsybakov (2018) for Gaussian regression, \( \hat{\eta}_{gL} \) with \textit{adaptively} chosen \( \lambda \) can achieve the minimax rate in the latter case as well but the proof of this conjecture is beyond the scope of the paper.

2. Variable \( \lambda_j \)'s. Consider

\[
\lambda_j = C_1 \sqrt{\frac{L + \ln(d/j)}{n}}
\]

that evidently satisfies (14). One can also verify that

\[
\sum_{j=1}^{d_0} \sqrt{\frac{L + \ln(d/j)}{j}} \leq \frac{2L}{L-1} \sqrt{d_0(L + \ln(d/d_0))} \leq 4 \sqrt{d_0 \left( L - 1 + \ln \left( \frac{d}{d_0} \right) \right)}
\]

Theorem \textsection 4 implies then:

**Corollary 2.** Consider a \( d_0 \)-sparse multinomial logistic regression (1)-(2). Apply the multinomial logistic group Slope classifier (13) with \( \lambda_j \)'s from (16).

Then, under Assumptions (A) and (B),

\[
\sup_{\eta^* \in C_L(d_0)} \mathcal{E}(\hat{\eta}_{gS}, \eta^*) \leq C(\delta) \left( \frac{d_0(L - 1) + d_0 \ln \left( \frac{d}{d_0} \right)}{n} \right)^{\frac{\alpha+1}{\alpha+2}}
\]

for all \( 1 \leq d_0 \leq \min(d, n) \) and all \( \alpha \geq 0 \).

Hence, the multinomial logistic group Slope classifier with variable \( \lambda_j \)'s from (16) is adaptively rate-optimal for both small and large number of classes, and, unlike the penalized likelihood estimator \( \hat{\eta}_{g\hat{M}} \), is computationally feasible.

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**References**

[1] Abramovich, F. and Grinshtein, V. (2010). MAP model selection in Gaussian regression. \textit{Electr. J. Statist.} 4, 932–949.

[2] Abramovich, F. and Grinshtein, V. (2016). Model selection and minimax estimation in generalized linear models. \textit{IEEE Trans. Inf. Theory} 62, 3721–3730.
[3] Abramovich, F. and Grinshtein, V. (2019). High-dimensional classification by sparse logistic regression. *IEEE Trans. Inf. Theory* 65, 3068–3079.

[4] Agarwal, A. (2013). Selective sampling algorithms for cost-sensitive multiclass prediction. *Proc. 30th Int. Conf. on Machine Learning, PMLR* 28(3), 1220–1228.

[5] Alquier, P., Cottet, V. and Lecué, G. (2019). Estimation bounds and sharp oracle inequalities of regularized procedures with Lipschitz loss functions. *Ann. Statist.* 47, 2117-2144.

[6] Ávila Pires, B., Szepesvári, C. and Ghavamzadeh, M. (2013). Cost-sensitive multiclass classification risk bounds. *Proc. 30th Int. Conf. on Machine Learning, PMLR* 28(3), 1391–1399.

[7] Ávila Pires, B. and Szepesvári, C. (2016). Multiclass classification calibration functions. arXiv:1609.06385.

[8] Bartlett, P.L., Jordan, M.I. and McAuliffe, J.D. (2006). Convexity, classification, and risk bounds. *J. Amer. Statist. Assoc.* 101, 138–156.

[9] Bellec, P.C., Lecué, G. and Tsybakov, A. (2018). Slope meets Lasso: improved oracle bounds and optimality. *Ann. Statist.* 46, 3603–3642.

[10] Bickel, P. and Levina, E. (2004). Some theory for Fisher’s discriminant function, ‘naive Bayes’, and some alternatives where there are more variables than observations. *Bernoulli*, 10, 989-1010.

[11] Bickel, P., Ritov, Y. and Tsybakov, A. (2009). Simultaneous analysis of Lasso and Dantzig selector. *Ann. Statist.* 37, 1705–1732.

[12] Birgé, L. and Massart, P. (2001). Gaussian model selection. *J. Eur. Math. Soc.* 3, 203–268.

[13] Bogdan, M., van den Berg, E., Sabatti, C., Su, W. and Candés, E. (2015). SLOPE – adaptive variable selection via convex programming. *Ann. Appl. Statist.*, 9, 1103–1140.

[14] Boucheron, S., Bousquet, O., and Lugosi, G. (2005). Theory of classification: a survey of some recent advances. *ESAIM: Prob. Statist.* 9, 323-375.

[15] Bunea, F., Tsybakov, A. and Wegkamp, M.H. (2007). Aggregation for Gaussian regression. *Ann. Statist.* 4, 1674–1697.

[16] Chen, D.-R. and Sun, T. (2006). Consistency of multiclass empirical risk minimization methods based on convex loss. *J. Mach. Learn. Res.* 7, 2435–2447.

[17] Danieli, A., Sabato, S. and Shalev-Shwartz, S. (2012). Multiclass learning approaches: a theoretical comparison with implications. *NIPS’12 Proceedings*, 485–493.
[18] Danieli, A., Sabato, S., Ben-David, S. and Shalev-Shwartz, S. (2015). Multiclass learnability and the ERM principle. *J. Mach. Learn. Res.* **16**, 2377–2404.

[19] Devroye, L., Györfi, L. and Lugosi, G. (1996). *A Probabilistic Theory of Pattern Recognition*. Springer, New York.

[20] Fan, J. and Fan, Y. (2008). High-dimensional classification using feature annealed independence rules. *Ann. Statist.* **36**, 2605–2637.

[21] Kesten, H. and Morse, N. (1959). A property of the multinomial distribution. *Ann. Math. Statist.* **30**, 120–127.

[22] Lecué, G. and Mendelson, S. (2018). Regularization and the small-ball method I: sparse recovery. *Ann. Statist.*, **46**, 611–641.

[23] Mammen, E. and Tsybakov, A. (1999). Smooth discrimination analysis. *Ann. Statist.* **27**, 1808–1829.

[24] Maurer, A. (2016). A vector-contraction inequality for Rademacher complexities. In: Ortner R., Simon H., Zilles S. (eds) *Algorithmic Learning Theory. ALT 2016. Lecture Notes in Computer Science* vol **9925**, Springer, Cham, 3–17.

[25] Maximov, Yu. and Reshetova, D. (2016). Tight risk bounds for multi-class margin classifiers. *J. Pattern Recogn. Image Analysis* **26**, 673–680.

[26] McCullagh, P. and Nelder, J. A. (1989). *Generalized Linear Models*, 2nd ed. Chapman and Hall, London.

[27] Natarajan, B.K. (1989). On learning sets and functions. *Mach. Learn.* **4**, 67-97.

[28] Rudelson, M. and Vershynin, R. (2013). Hanson-Wright inequality and sub-gaussian concentration. *Electron. Commun. Probab.* **18** (2013), 1-9.

[29] Su, W. and Candés, E.J. (2015). SLOPE is adaptive to unknown sparsity and asymptotically minimax. *Ann. Statist.* **44**, 1038–1068.

[30] Tewari, A. and Bartlett, P. L. (2007). On the consistency of multiclass classification methods. *J. Mach. Learn. Res.* **8**, 1007-1025.

[31] Tsybakov, A. (2004). Optimal aggregation of classifiers in statistical learning. *Ann. Statist.* **32**, 135–166.

[32] van de Geer, S. (2008). High-dimensional generalized linear models and the Lasso. *Ann. Statist.* **36**, 614–645.
Appendix

Throughout the proofs we use various generic positive constants, not necessarily the same each time they are used even within a single equation.

We first introduce several notations that will be used throughout the proofs. Let $|a|_2$ be the Euclidean norm of a vector $a$, $|A|_2$ the operator norm of a matrix $A$ and $|A|_F$ its Frobenius norm. Denote $||g||_{L_2} = (\int_X g^2(x) dx)^{1/2}$ for a standard $L_2$-norm of a function $g$ and $||g||_{L_2(P_X)} = (\int_X g^2(x) dP_X(x))^{1/2}$ for the $L_2$-norm of $g$ weighted w.r.t. the marginal distribution $P_X$ of $X$. In addition, the $L_\infty$-norm $||g||_\infty = \sup_{x \in X} |g(x)|$.

Proof of Theorem 2

It is obvious that feature selection and classification in multiclass case cannot be simpler than in binary. Formally, binary logistic classification may be viewed as a degenerate case of multinomial logistic classification with $L > 2$, where without loss of generality $p_l = 0$, $l = 2, \ldots, L - 1$ corresponding to $\beta_l = -\infty$, $l = 2, \ldots, L - 1$ (see Section 2.1). Define then a subset $\tilde{C}_L(d_0) = \{\eta(x) \in C_L(d_0) : \beta_l = -\infty, l = 2, \ldots, L - 1\}$. Thus,

$$\inf_{\tilde{\eta}} \sup_{\eta^* \in \tilde{C}_L(d_0), P_X} \mathcal{E}(\tilde{\eta}, \eta^*) \geq \inf_{\tilde{\eta}} \sup_{\eta^* \in \tilde{C}_L(d_0), P_X} \mathcal{E}(\tilde{\eta}, \eta^*) = \inf_{\tilde{\eta}} \sup_{\eta^* \in C_2(d_0), P_X} \mathcal{E}(\tilde{\eta}, \eta^*)$$

and using the results of Abramovich and Grinshtein (2019, Section 6) for binary classification we have $\inf_{\tilde{\eta}} \sup_{\eta^* \in C_2(d_0), P_X} \mathcal{E}(\tilde{\eta}, \eta^*) > C \sqrt{\frac{d_0 \ln \frac{d_0}{n}}{n}}$ for some $C > 0$.

On the other hand, for a given model $M$ of size $d_0$, consider the corresponding set of $d_0$-dimensional linear $L$-class classifiers $C^M_L = \{\eta(x) \in C_L(d_0) : B \in \mathcal{B}_M\}$. Obviously, $\inf_{\tilde{\eta}} \sup_{\eta^* \in C_L(d_0), P_X} \mathcal{E}(\tilde{\eta}, \eta^*) \geq \inf_{\tilde{\eta}} \sup_{\eta^* \in C^M_L, P_X} \mathcal{E}(\tilde{\eta}, \eta^*)$. From the general results of Theorem 5 of Daniely et al. (2015), it follows
implies that under the low-noise condition (10)-(11),
\[ \delta \text{ with the calibration function } \logistic \text{ corresponding to the logistic surrogate loss and applying then their Theorem 3.11 and Szepesvári (2016) among many others.} \]

and, therefore,
\[ d \text{ and } \delta. \]

Yang and Barron (1998) and then apply their Theorem 1 to find an upper bound for the bounds of some related surrogate risk (see Section 1) which can be established by various existing methods. See, e.g., Zhang (2004ab), Bartlett, Jordan and McAuliffe (2006), Ávila Pires and Lugosi, 1996, Chapter 14).

To complete the proof we use the bounds for Natarajan dimension of the set of \( d_0 \)-dimensional linear \( L \)-class classifiers established in Daniely et al. (2012, Theorem 3.1), namely, \( d_0(L - 1) \leq d_N(C_L^M) \leq O(d_0 \ln(d_0L)). \)

### Proof of Theorem 3

Let \( KL(p_1, p_2) = \sum_{l=1}^{L} p_l \ln \left( \frac{p_l}{p_l} \right) \) and \( H^2(p_1, p_2) = \frac{1}{2} \sum_{l=1}^{L} (\sqrt{p_{l1}} - \sqrt{p_{l2}})^2 \) be respectively the Kullback-Leibler divergence and the square Hellinger distance between two multinomial distributions with success probabilities vectors \( p_1 \) and \( p_2 \). Let also \( d_{KL}(f_{B_1}, f_{B_2}) = \int KL(p_1(x), p_2(x))dP_X(x) \) and \( d_H^2(f_{B_1}, f_{B_2}) = \int H^2(p_1(x), p_2(x))dP_X(x) \) be the corresponding Kullback-Leibler divergence and square Hellinger distance between \( f_{B_1} \) and \( f_{B_2} \).

One can verify that for \( p_1 \) and \( p_2 \) satisfying Assumption (A), \( KL(p_1, p_2) \leq \frac{4(1-\delta)^2}{\alpha} H^2(p_1, p_2) \) and, therefore, \( d_{KL}(f_{B_1}, f_{B_2}) \leq \frac{4(1-\delta)^2}{\alpha} d_H^2(f_{B_1}, f_{B_2}) \).

A common approach to derive the upper bounds for misclassification risk is to convert them to the bounds of some related surrogate risk (see Section 1) which can be established by various existing methods. See, e.g., Zhang (2004ab), Bartlett, Jordan and McAuliffe (2006), Ávila Pires and Szepesvári (2016) among many others.

Thus, utilizing the results of Section 5.2 of Ávila Pires and Szepesvári (2016) for multiclass logistic regression corresponding to the logistic surrogate loss and applying then their Theorem 3.11 with the calibration function \( \delta'(\epsilon) = 0.5 ((1-\epsilon) \ln(1-\epsilon) + (1+\epsilon) \ln(1+\epsilon)) \geq 0.5\epsilon^2 \) and \( \alpha' = \frac{\alpha}{\alpha+1} \) implies that under the low-noise condition (10)-(11),
\[ E(\tilde{\eta}_{M}, \eta^*) \leq C \left( Ed_{KL}(f_B, f_{B_{\tilde{M}}}) \right)^{\frac{\alpha+1}{\alpha+2}} \leq C \left( \frac{1}{\delta^2} Ed_H^2(f_B, f_{B_{\tilde{M}}}) \right)^{\frac{\alpha+1}{\alpha+2}} \]

and it is, therefore, sufficient to bound the square Hellinger risk \( Ed_H^2(f_B, f_{B_{\tilde{M}}}) \).

We will show now that the penalty [7] falls within a general class of penalties considered in Yang and Barron (1998) and then apply their Theorem 1 to find an upper bound for \( Ed_H^2(f_B, f_{B_{\tilde{M}}}) \).

It is easy to verify that
\[ H^2(p_1, p_2) \geq \frac{1}{8} |p_1 - p_2|^2 \]

and
\[ d_N(C_L^M) \leq O(d_0 \ln(d_0L)). \]
Furthermore, using the standard inequality $\ln(1 + t) \leq t$, under Assumption (A) we have

$$
|\ln f_{B_2}(x, y) - \ln f_{B_1}(x, y)| = \left| \sum_{l=1}^{L} \xi_l \ln \frac{p_{2l}(x)}{p_{1l}(x)} \right| \leq \max_{1 \leq l \leq L} \left| \ln \frac{p_{2l}(x)}{p_{1l}(x)} \right|
\leq \frac{1}{\delta} \max_{1 \leq l \leq L} |p_{2l}(x) - p_{1l}(x)|,
$$

where recall that $\xi \in \{0, 1\}^L$ is the indicator vector assigned to $y$.

Define $\rho(f_{B_1}, f_{B_2}) = ||\ln f_{B_2} - \ln f_{B_1}||_\infty$. Thus,

$$
\rho(f_{B_1}, f_{B_2}) \leq \frac{1}{\delta} \max_{1 \leq l \leq L} ||p_{2l} - p_{1l}||_\infty \tag{20}
$$

For a given model $M$ consider the set of coefficient matrices $B_M$ defined in Section 2.2. One can easily verify that under Assumption (A), for any $B_1, B_2 \in B_M$ with columns $\beta_1$’s and $\beta_2$’s respectively and the corresponding probability vectors $p_1(x), p_2(x)$

$$
\delta(1 - \delta)  \langle (\beta_2 - \beta_1)^t x \rangle \leq |p_{2l}(x) - p_{1l}(x)| \leq \frac{1}{4} |(\beta_2 - \beta_1)^t x| \tag{21}
$$

for all $l = 1, \ldots, L - 1$ and any $x \in X$.

In particular, (21) implies

$$
\sum_{l=1}^{L} ||p_{2l} - p_{1l}||_2^2 (p_x) \geq \delta^2 (1 - \delta)^2 \sum_{l=1}^{L} (\beta_2 - \beta_1)^t G(\beta_2 - \beta_1) \geq \delta^2 (1 - \delta)^2 \lambda_{\min}(G) |B_2 - B_1|^2_F \tag{22}
$$

(recall that $\beta_{1L} = \beta_{2L} = 0$).

For each matrix $B_0 \in B_M$ consider the corresponding Hellinger ball $H_{f_{B_0}, r} = \{ f_B : d_H(f_B, f_{B_0}) \leq r, B \in B_M \}$. From (19) and (22) it then follows that if $f_B \in H_{f_{B_0}, r}$, the corresponding $B \in B_M$ lies in the Frobenius ball $B_{B_0, r'} = \{ B \in \mathbb{R}^{M|X|L} : |B - B_0|_F \leq r' \}$ with $r' = \frac{2r}{\delta(1 - \delta) \sqrt{\lambda_{\min}(G)}}$.

Furthermore, for any $|x|_2 \leq 1$ and any $1 \leq l \leq L - 1$, (21) and Cauchy-Schwarz inequality imply that $|p_{2l}(x) - p_{1l}(x)| \leq \frac{1}{4} |\beta_2 - \beta_1|_2$ and, therefore,

$$
\max_{1 \leq l \leq L - 1} ||p_{2l} - p_{1l}||_\infty \leq \frac{1}{4} \max_{1 \leq l \leq L - 1} |\beta_2 - \beta_1|_2 \leq \frac{1}{4} \sqrt{\sum_{l=1}^{L} |\beta_2 - \beta_1|_2^2} = \frac{1}{4} |B_2 - B_1|_F
$$

Then, by (20)

$$
\rho(f_{B_1}, f_{B_2}) \leq \frac{1}{4\delta} |B_2 - B_1|_F \tag{23}
$$

Let $N(B_{B_0, r'}, F, \epsilon)$ be the $\epsilon$-covering number of $B_{B_0, r'}$ w.r.t. the Frobenius distance. Note that the Frobenius norm of a $|M| \times L$ matrix with zero last column is equivalent to the Euclidean norm of a vector of its entries of the first $(L - 1)$ columns. We can use then the well-known results for the covering number of an Euclidean ball in $\mathbb{R}^{(L-1)|M|}$ to have $N(B_{B_0, r'}, F, \epsilon) \leq \left(1 + \frac{2r'}{\epsilon}\right)^{(L-1)|M|} \leq \left(\frac{3r'}{\epsilon}\right)^{(L-1)|M|}$ for any $\epsilon < r'$. 

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Thus, for the \( \epsilon \)-covering number \( N(\mathcal{H}_{f_{B_0},r}, \rho, \epsilon) \) of \( \mathcal{H}_{f_{B_0},r} \) w.r.t. the distance \( \rho(f_{B_1}, f_{B_2}) \), from (23) we have

\[
N(\mathcal{H}_{f_{B_0},r}, \rho, \epsilon) \leq N(\mathcal{B}_{B_0,r^*}, F, 4\delta \epsilon) \leq \left( \frac{6}{4\delta^2(1-\delta)\sqrt{\lambda_{\min}(G)}} \right)^{(L-1)|M|} r \epsilon^{-1}
\]

The considered family of sparse multinomial logistic regression models satisfies then Assumption 1 of Yang and Barron (1998) with \( A_M = \frac{c}{\delta^2(1-\delta)\sqrt{\lambda_{\min}(G)}} \) for some \( c > 0 \) and \( m_M = (L-1)|M| \). Apply now their Theorem 1 for a penalized maximum likelihood model selection procedure (5) with a complexity penalty \( \text{Pen}(|M|) = C_1 m_M \ln A_M + C_2 \cdot C_M \leq C_1 (L-1)|M| + C_2 |M| \ln \left( \frac{d e}{|M|} \right) \), where \( C_M = |M| \ln \left( \frac{d e}{|M|} \right) \), and the exact positive constants \( C_1 \) and \( C_2 \) are given in their paper. Thus,

\[
Ed_H^2(f_{\bar{B}_M^S}, f_B) \leq C(\delta, \lambda_{\min}(G)) \frac{\text{Pen}(d_0)}{n} \leq C(\delta, \lambda_{\min}(G)) \frac{(L-1)d_0 + \ln \left( \frac{d e}{d_0} \right)}{n}
\]

that together with (18) complete the proof.

**Proof of Theorem 4**

First, recall that from (18) it follows that

\[
E(\hat{\eta}_{gS}, \eta^*) \leq C \left( Ed_{KL}(f_B, f_{\hat{gS}^S}) \right)^{\frac{\alpha+1}{\alpha+2}}
\]

and, thus, it is sufficient to bound the Kullback-Leibler risk \( Ed_{KL}(f_B, f_{\hat{gS}^S}) \). For this purpose, we extend the corresponding results of Alquier, Cottet and Lecué (2019) for logistic Slope to its group analogue in multinomial logistic regression model.

As we have mentioned, the solution of (13) satisfies the symmetric constraint \( \sum_{l=1}^L \beta_{gS,l} = 0 \). Let \( \theta_l(x) = \beta_l^T x \), \( l = 1, \ldots, L \) with the constraint \( \sum_{l=1}^L \theta_l(x) = 0 \). Thus, \( \theta_l(x) = \theta_l(x)/\sum_{l'=1}^L e^{\theta_{l'}(x)} \) and in terms of \( \theta(x) \), the likelihood (3) is \( \ell(\theta(x)) = \sum_{l=1}^L \theta_l(x) - \ln \left( \sum_{l'=1}^L e^{\theta_{l'}(x)} \right) \) which is Lipschitz with constant 2, i.e. \( |\ell(\theta_1(x)) - \ell(\theta_2(x))| \leq 2|\theta_1(x) - \theta_2(x)|_2 \). Furthermore, similar to Lemma 1 of Abramovich and Grinshtein (2016) for binary logistic regression, re-writing the Kullback-Leibler divergence \( KL(p_1(x), p_2(x)) \) in terms of \( \theta(x) \) and expanding it in (multivariate) Taylor series, one can verify that under Assumption (A), \( KL(\theta_1(x), \theta_2(x)) \geq \frac{1}{2\delta^2} |\theta_1(x) - \theta_2(x)|_2^2 \) and, therefore, \( d_{KL}(f_{B_1}, f_{B_2}) \geq \frac{1}{2\delta^2} \sum_{l=1}^L \|\theta_{l1}(x) - \theta_{l2}(x)\|_2^2 \) (a multivariate analogue of Bernstein condition in terminology of Alquier, Cottet and Lecué, 2019). Lipschitz and Bernstein conditions allow us to apply the general approach of Alquier, Cottet and Lecué (2019) and to extend their results to multinomial logistic group Lasso and group Slope. In particular, Assumption (A) corresponds to the bounded case considered there.

Let \( B \) be a set of matrices \( B \) satisfying the symmetric constraint, i.e. \( B = \{ B \in \mathbb{R}^{d \times L} : B1 = 0 \} \). For a given regression coefficients matrix \( B \in B \) with (zero mean) rows \( B_j \), define its group Slope
norm $|B|_\lambda = \sum_{j=1}^d \lambda_j |B|_{(j)}$, where recall that $|B|_{(1)} \geq \ldots \geq |B|_{(d)}$ are the descendingly ordered $l_2$-norms of $B_j$’s, and consider the corresponding unit ball $B_\lambda$.

To derive an upper bound on $E d_{KL}(f_B, f_{\tilde{B}})$ we define the following quantities along the lines of Alquier, Cottet and Lecué (2019).

Let $Rad(B_\lambda)$ be the Rademacher complexity of $B_\lambda$, namely,

$$ Rad(B_\lambda) = E \frac{1}{\sqrt{n}} \sup_{B \in B_\lambda} \sum_{i=1}^n \sum_{l=1}^L \sigma_{il} \beta_l x_i = E \frac{1}{\sqrt{n}} \sup_{B \in B_\lambda} tr(\Sigma B^t X^t), $$

where the elements $\sigma_{il}$’s of $\Sigma \in \mathbb{R}^{n \times L}$ are i.i.d. Rademacher random variables with $P(\sigma_{il} = 1) = P(\sigma_{il} = -1) = 1/2$.

Define a complexity function

$$ r(\rho) = \sqrt{\frac{C_0 Rad(B_\lambda) \rho}{2\delta^2 \sqrt{n}}}, \quad \rho > 0, $$

where the exact value of $C_0 > 0$ is specified in Alquier, Cottet and Lecué (2019).

Let $\mathcal{M}(\rho) = \{B \in \mathcal{B} : |B|_\lambda = \rho, \sum_{l=1}^L ||B^t_l x||_{l_2} \leq r^2(2\rho)\}$. For a given matrix $B \in \mathcal{B}$ define $\Gamma_B(\rho) = \bigcup_{B' : B, B' \in \mathcal{B}, |B'| = \lambda} \{B' \in \mathcal{B} : |B' - B|_\lambda < 2\delta \cdot |\lambda(B') = \{B'' \in \mathcal{B} : |B' + B''|_\lambda - |B'|_\lambda \geq tr((B')^t B'')\}$. The sparsity parameter is

$$ \Delta(\rho) = \inf_{B' \in \mathcal{M}} \sup_{H \in \Gamma_B(\rho)} <H, B> = \inf_{B' \in \mathcal{M}} \sup_{H \in \Gamma_B(\rho)} tr(H^t B') $$

Let $B \in \mathcal{B}$ be $d_0$-sparse and define

$$ \rho^* = \frac{C_0}{800\delta^2} \frac{Rad(B_\lambda) \left(\sum_{j=1}^{d_0} \lambda_j / \sqrt{j}\right)}{\sqrt{n}} \tag{24} $$

A straightforward extension of Lemma 4.3 of Lecué and Mendelson (2018) for matrices implies that $\Delta(\rho^*) > \frac{4}{5}\rho^*$ and, therefore, we can apply the following Lemma 1, which can be viewed as an extension of Theorem 2.2 (or more general Theorem 9.2) of Alquier, Cottet and Lecué (2019) for our case:

**Lemma 1.** Let $B \in \mathcal{B}$ be $d_0$-sparse and let $\lambda_j$’s be such that $Rad(B_\lambda) \leq \frac{7}{200}\delta \sqrt{n}$. If $\rho^*$ defined in (24) satisfies $\Delta(\rho^*) > \frac{4}{5}\rho^*$, then

$$ Ed_{KL}(f_B, f_{\tilde{B}}) \leq C(\delta) \left(\sum_{j=1}^{d_0} \frac{\lambda_j}{\sqrt{j}}\right)^2 \tag{25} $$

for some constant $C(\delta)$ depending on $\delta$.

To satisfy the conditions of Lemma 1 and to complete the proof, we need to find an upper bound for the Rademacher complexity $Rad(B_\lambda)$:
Lemma 2.

\[
\text{Rad}(B_\lambda) \leq C_0 \max_{1 \leq j \leq d} \sqrt{L + \ln \left( \frac{d}{j} \right) \lambda_j},
\]

where the exact constant \( C_0 \) is given in the proof.

Proof of Lemma 1

The proof is an extension of the proof of Theorem 9.2 in the supplementary material of Alquier, Cottet and Lecué (2019) for the multiclass framework. In a slightly more general version of Proposition 9.1 of Alquier, Cottet and Lecué (2019) we define the following event \( \Omega_{t0} \) for \( t \geq 1 \):

\[
\Omega_{t0} = \left\{ \forall B' \in \mathcal{B}, \left| \frac{1}{n}(\ell(B') - \ell(B)) - \mathbb{E}[(\ell(B') - \ell(B))] \right| \leq \frac{7}{20} \delta^2 \max \left( r(2 \max (|B' - B|_\lambda, t\rho^*))^2, \sum_{i=1}^{L} ||(B_i - B_i')^x||_{L^2}^2 \right) \right\}.
\]

(Proposition 9.1 of Alquier, Cottet and Lecué 2019 considers only \( \Omega_0^1 \)).

As stated above, Assumption (A) implies the required Bernstein condition. The condition \( \text{Rad}(B_\lambda) \leq \frac{7}{20} \sqrt{n} \) is needed for adjusting the scale of the norm w.r.t. to the loss required in Theorem 9.2 of Alquier, Cottet and Lecué (2019). Under these two conditions, we can follow the proof of Proposition 9.1 of Alquier, Cottet and Lecué (2019) to get

\[
d_{KL}(f_B, f_{B^*_S}) \leq 2\delta^2 r (2\rho^*)^2 \leq C\rho^* \text{Rad}(B_\lambda) \sqrt{n}.
\]

on the event \( \Omega_0^1 \).

To extend the proof for \( t > 1 \), note that \( t\rho^* \geq \rho^* \). Since \( \Delta(\rho^*) \geq \frac{2}{3} \rho^* \), when \( |B' - B|_\lambda \geq t\rho^* \geq \rho^* \) we still have \( \Delta(|B' - B|_\lambda) \geq \frac{4}{3} |B - B^*|_\lambda \) (see Lemma A.1 in Alquier, Cottet and Lecué, 2019). Thus, following the arguments of Proposition 9.1, on the event \( \Omega_{t0}^1 \) we have

\[
d_{KL}(f_B, f_{B^*_S}) \leq 2\delta^2 r (2\rho^*)^2 t \leq C\rho^* \text{Rad}(B_\lambda) \sqrt{n} t.
\]

To bound the probability of \( \Omega_{t0}^1 \), we follow Proposition 9.3 of Alquier, Cottet and Lecué (2019). We consider the subsets \( F_{j,i} = \left\{ B : \rho_{j-1} \leq |B' - B|_\lambda \leq \rho_j, r_i-1(\rho_j) \leq \sum_{i=1}^{L} ||(B_i - B_i')^x||_{L^2} \leq r_i(\rho_j) \right\} \), where \( \rho_j = 2^j \rho^* \) and \( r_i(\rho) = 2^i r(\rho) \), \( i, j = 0,1, \ldots \).

Replace \( \rho_j \) with \( t\rho_j \) and go along the lines of the proof of Proposition 9.3 of Alquier, Cottet and Lecué (2019) with the extended contraction inequality for Rademacher complexities for vector-valued Lipschitz functions of Maurer (2016) to get

\[
P(\Omega_{t0}^1) \geq 1 - 2 \sum_{j=0}^{\infty} \sum_{i \in I_j} \exp \left( -\frac{1}{48} \tilde{C}(\delta) \frac{7}{20} \delta^2 n (2^i r (t2^j \rho^*))^2 \right).
\]
Recall that $B \mathbf{1} = \mathbf{0}$ for $B \in \mathcal{B}$. Define the matrix $U \in \mathbb{R}^{L \times (L-1)}$ which (orthonormal) columns are the $L - 1$ eigenvectors of the matrix $I_L - \frac{1}{L} \mathbf{1} \mathbf{1}^t$ corresponding to the eigenvalue 1. One can easily verify that $B = BUU^t$. Then,

$$Rad(B_\lambda) = \sup_{B \in \mathcal{B}_\lambda} tr(\Sigma B^t \mathbf{x}^t) = \sup_{B \in \mathcal{B}_\lambda} tr(\mathbf{X}^t \Sigma UU^t B^t) = \sup_{B \in \mathcal{B}_\lambda} tr(K^t UU^t B^t) = \sup_{B \in \mathcal{B}_\lambda} \sum_{j=1}^d K_j^1 U^t B_j,$$

Substituting $\rho^*$ from (24) into (27) under the conditions of the lemma completes the proof.

**Proof of Lemma 2**

Recall that $B \mathbf{1} = \mathbf{0}$ for $B \in \mathcal{B}$. Define the matrix $U \in \mathbb{R}^{L \times (L-1)}$ which (orthonormal) columns are the $L - 1$ eigenvectors of the matrix $I_L - \frac{1}{L} \mathbf{1} \mathbf{1}^t$ corresponding to the eigenvalue 1. One can easily verify that $B = BUU^t$. Then,

$$Rad(B_\lambda) = \sup_{B \in \mathcal{B}_\lambda} tr(\Sigma B^t \mathbf{x}^t) = \sup_{B \in \mathcal{B}_\lambda} tr(\mathbf{X}^t \Sigma UU^t B^t) = \sup_{B \in \mathcal{B}_\lambda} tr(K^t UU^t B^t) = \sup_{B \in \mathcal{B}_\lambda} \sum_{j=1}^d K_j^1 U^t B_j,$$
where \( K = U^t \Sigma^t X \). Let \(|K|_j = |K_j|_2\). By Cauchy-Schwartz inequality and the definition of the group Slope norm \( |B|_\lambda \), we have

\[
\sup_{B \in B_\lambda} \sum_{j=1}^d K_j^t U B_j \leq \sup_{B \in B_\lambda} \sum_{j=1}^d |(UB)_j|_2 \cdot |K_j|_2 = \sup_{B \in B_\lambda} \sum_{j=1}^d |B_j| \cdot |K_j| \leq \sup_{B \in B_\lambda} \sum_{j=1}^d \lambda_j |B_j| \cdot \frac{|K_j|}{\lambda_j} \leq \max_{1 \leq j \leq d} \frac{|K_j|}{\lambda_j}
\]

Thus, \( \text{Rad}(B_\lambda) \leq E \max_{1 \leq j \leq d} \frac{1}{\sqrt{n}} \frac{|K_j|}{\lambda_j} \).

Let \( x_j^* = \frac{x_j}{|x_j|_2} \) be normalized columns of \( X \). Then, \( \frac{1}{\sqrt{n}} K_j = A_j \Sigma^t x_j^* \), where the matrix \( A_j = \frac{|x_j|^2}{\sqrt{n}} U^t \). Note that \( |A_j|_F^2 = \frac{1}{n} |x_j|_2^2 (L - 1) \leq L - 1 \) and \( |A_j|_2 = \frac{1}{\sqrt{n}} |x_j| \leq 1 \). We can apply then the results of Rudelson and Vershynin (2013, p.8) to get

\[
P \left( \frac{1}{\sqrt{n}} |K|_j \geq t \sqrt{L + \ln(d/j)} \right) = P \left( \frac{1}{\sqrt{n}} |K|_j \geq t \sqrt{L - 1 + \ln \left( \frac{de}{j} \right)} \right) \leq P \left( \frac{1}{\sqrt{n}} |K|_j \geq \frac{t}{\sqrt{2}} \sqrt{L - 1 + \frac{t}{\sqrt{2}} \ln \left( \frac{de}{j} \right)} \right) \leq P \left( \frac{1}{\sqrt{n}} |K|_j \geq \frac{t}{\sqrt{2}} \frac{\sqrt{L - 1}}{\lambda_j} \right) \leq 2e^{- \frac{ct^2 \ln(\frac{de}{j})}{2}} \leq 2 \left( \frac{de}{j} \right)^{-ct^2}
\]

for all \( t \geq \sqrt{2} \) and a certain constant \( c > 0 \).

Hence, by standard probabilistic arguments, for all \( t \geq \max(\sqrt{2}, \frac{2}{\sqrt{c}}) \)

\[
P \left( \frac{1}{\sqrt{n}} \frac{|K|_j}{\lambda_j} > t \frac{\sqrt{L + \ln(d/j)}}{\lambda_j} \right) \leq 2 \left( \frac{de}{j} \right)^{-jct^2} \leq 2 \left( \frac{de}{j} \right)^{-jc^2 t^2} \leq 2 \left( \frac{de}{j} \right)^{-jc^2 t^2}
\]

and applying the union bound,

\[
P \left( \frac{1}{\sqrt{n}} \max_{1 \leq j \leq d} \frac{|K|_j}{\lambda_j} > t \max_{1 \leq j \leq d} \frac{\sqrt{L + \ln(d/j)}}{\lambda_j} \right) \leq \sum_{j=1}^d P \left( \frac{1}{\sqrt{n}} \frac{|K|_j}{\lambda_j} > t \frac{\sqrt{L + \ln(d/j)}}{\lambda_j} \right) \leq 2 \sum_{j=1}^d \left( \frac{de}{j} \right)^{-jc^2 t^2} \leq 2 \sum_{j=1}^d e^{-jc^2 t^2} \leq 2 \frac{e^{-c^2 t^2}}{1 - e^{-c^2 t^2}} \leq 4e^{-c^2 t^2}
\]

Therefore,

\[
E \left( \frac{1}{\sqrt{n}} \max_{1 \leq j \leq d} \frac{|K|_j}{\lambda_j} \right) = \int_0^\infty P \left( \frac{1}{\sqrt{n}} \max_{1 \leq j \leq d} \frac{|K|_j}{\lambda_j} > t \max_{1 \leq j \leq d} \frac{\sqrt{L + \ln(d/j)}}{\lambda_j} \right) dt \leq \max \left( \sqrt{2}, \frac{2}{\sqrt{c}} \right) + 4 \int_{\max(\sqrt{2}, \frac{2}{\sqrt{c}})}^\infty e^{-c^2 t^2} dt = C_0
\]

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