Group-regularized ridge regression via empirical Bayes noise level cross-validation

Nikolaos Ignatiadis∗ Panagiotis Lolas†

Draft manuscript: October 2020

Abstract
Features in predictive models are not exchangeable, yet common supervised models treat them as such. Here we study ridge regression when the analyst can partition the features into $K$ groups based on external side-information. For example, in high-throughput biology, features may represent gene expression, protein abundance or clinical data and so each feature group represents a distinct modality. The analyst’s goal is to choose optimal regularization parameters $\lambda = (\lambda_1, \ldots, \lambda_K)$ – one for each group. In this work, we study the impact of $\lambda$ on the predictive risk of group-regularized ridge regression by deriving limiting risk formulae under a high-dimensional random effects model with $p \asymp n$ as $n \to \infty$. Furthermore, we propose a data-driven method for choosing $\lambda$ that attains the optimal asymptotic risk: The key idea is to interpret the residual noise variance $\sigma^2$, as a regularization parameter to be chosen through cross-validation. An empirical Bayes construction maps the one-dimensional parameter $\sigma$ to the $K$-dimensional vector of regularization parameters, i.e., $\sigma \mapsto \hat{\lambda}(\sigma)$. Beyond its theoretical optimality, the proposed method is practical and runs as fast as cross-validated ridge regression without feature groups ($K = 1$).

1 Introduction

The predictive performance of supervised learning methods that predict a response $Y_i$ from high-dimensional features $x_i$ can be improved by using external knowledge about the features, i.e., side-information that is not contained in the numerical values of the $x_i$. For example, in high-throughput biology, the features may comprise of distinct modalities, such as gene expression, protein abundance or clinical data. The gene expression features in turn correspond to different genetic pathways or perhaps to the same genes measured across multiple tissues. Van De Wiel, Lien, Verlaat, van Wieringen, and Wilting [2016] use the term “co-data” for such external information, while Tay, Aghaeepour, Hastie, and Tibshirani [2020] use the term “features of features”. How can we use such side-information to improve predictive performance in a principled way?

The conceptual move away from exchangeable features to features with side-information is straight-forward. For continuous $Y_i \in \mathbb{R}$, $x_i \in \mathbb{R}^p$ $i = 1, \ldots, n$ consider the regularized regression,

$$\hat{w} = \inf_w \left\{ \frac{1}{2n} \sum_{i=1}^{n} (Y_i - x_i^\top w)^2 + \text{Pen}(w) \right\}.$$  

In the exchangeable setting, without a-priori information about the features, Pen$(w)$ is typically chosen as a symmetric regularizer, such as Pen$(w) = \lambda \|w\|_2^2 / 2$ [Hoerl and Kennard, 1970,}

∗Department of Statistics, Stanford University (ignat@stanford.edu)
†Department of Mathematics, Stanford University (panagd@stanford.edu)
We consider a situation in which the domain scientist can partition the features conceptually and empirically studying the simplest practically relevant form of (1) with feature co-data. The natural way then of accounting for feature side-information is to choose a regularizer $\text{Pen}(\mathbf{w})$ that is not symmetric. However, if one seeks to turn this conceptual extension into a practical method, one is immediately faced with a key difficulty: a Tikhonov, 1963] or $\text{Pen}(\mathbf{w}) = \lambda \|\mathbf{w}\|_1$ [Tibshirani, 1996] with the regularization parameter $\lambda$ tuned, say, through cross-validation. The solution to (2) with $\lambda^\star$ tuned, is \[
\hat{\mathbf{w}} = \hat{\mathbf{w}}(\mathbf{\lambda}) = \arg\min_{\mathbf{w}} \left\{ \frac{1}{2n} \sum_{i=1}^{n} (Y_i - x_i^\top \mathbf{w})^2 + \sum_{g=1}^{K} \frac{\lambda_g}{2} \|\mathbf{w}|_g\|_2^2 \right\}
\]
The issue, as already alluded, is the following: How should one choose the $K$-dimensional $\mathbf{\lambda} = (\lambda_1, \ldots, \lambda_K)$ needed to solve (2) and what is the impact of this choice? Our starting point for answering this question is the following generative model for the data: let $p_g = |G_g|$ the number of features in group $g$ and $\sigma > 0, \sigma_1^2, \ldots, \sigma_K^2 > 0$. Then generate (independently)
\[
\begin{align*}
  w_j &\sim \mathcal{N}(0, \sigma_g^2/p_g) & j \in G_g, \ g = 1, \ldots, K \\
  x_i &\sim \mathcal{P}^X, \ \varepsilon_i \sim \mathcal{N}(0, \sigma^2) \ \ Y_i = x_i^\top \mathbf{w} + \varepsilon_i & i = 1, \ldots, n 
\end{align*}
\]
Under model (3), we can precisely characterize the limiting risk of predictions $x \mapsto x^\top \hat{\mathbf{w}}(\mathbf{\lambda})$ for any value of $\mathbf{\lambda}$ by utilizing recent advances in random matrix theory (RMT), cf. Dobriban and Wager [2018] and thus we can study the impact of different choices of $\mathbf{\lambda}$. Furthermore, under (3), we can plausibly choose $\mathbf{\lambda} \in [0, \infty)^K$ with a fully model-based approach as we now explain. The solution to (2) with $\mathbf{\lambda}_g = \frac{p_g}{n} \frac{\sigma^2}{\sigma_g^2}$ is the posterior mean of $\mathbf{w}$ under model (3) and so one could fit (3) to estimate $\alpha = (\alpha_1, \ldots, \alpha_K)$ and $\sigma^2$, and then solve (2) with plug-in estimates of (4). This approach, however, comes with caveats: estimation typically proceeds by optimization of a non-convex objective, such as restricted maximum likelihood. Furthermore, a data scientist interested in predictive performance may be apprehensive of choosing parameters based on purely model-based criteria. Instead, they may prefer to directly optimize distribution-free measures of predictive performance. For example, they may choose $\mathbf{\lambda} \in [0, \infty)^K$ by minimizing the cross-validated mean squared error. For small $K$, this may be achieved by exhaustive grid search, otherwise, one would resort to heuristics for the optimization of non-convex objectives.

The methodological contribution of this paper is the development of $\sigma$-Ridge regression, a hybrid of the two aforementioned approaches – model-based tuning and cross-validation – with several favorable properties, which we outline next.

1. **Single regularization parameter**: $\sigma$-Ridge regression depends on a single, interpretable regularization parameter, which can be chosen by cross-validation. The data scientist can inspect parameter and coefficient paths as a function of the regularization parameter.

2. **Computationally tractable**: The method has the same computational complexity as cross-validated Ridge regression with a single $\lambda$. All underlying computations may be solved to machine precision without any danger of local minima.
Figure 1: $\sigma$-Ridge regression: We apply $\sigma$-Ridge regression to a single simulation from model (3) with $x_i \sim \mathcal{N}(0, I)$, $n = 400$, $K = 3$, $p_g = 25$, $\omega_g^2 = 4 \cdot g$ and $\sigma^2 = 16$. **Panel a)** shows the map $\sigma \mapsto \hat{\lambda}(\sigma)$ from $\sigma$ to the per-group regularization parameter. The first group, with the lowest signal, receives the largest penalty. As $\sigma$ increases, we regularize more aggressively. **Panel b)** shows the leave-one-out cross-validation error $\text{CV}^\ast(\sigma)$ as a function of $\sigma$. The minimizer of the curve can be used as a data-driven choice for $\sigma$.

3. **Asymptotic Optimality in high dimensions:** The method provably matches the predictive performance of the best estimator in the class (2) in a high-dimensional nonparametric random effects model that generalizes (3). Under the same model, $\sigma$-Ridge regression also provably outperforms the Group Lasso [Yuan and Lin, 2006] with optimal tuning\(^1\).

4. **Practical:** The method works well in practical situations and datasets, wherein model (3) may not hold.

1.1 How does $\sigma$-Ridge regression work?

The key idea of our proposal is that it is possible to develop a hybrid of cross-validation and model-based hyperparameter tuning. Assume momentarily **a)** that model (3) holds and **b)** that $\sigma$ is known to the analyst. Then let $\hat{\alpha}(\sigma)$ be a model-based estimate (more of which in Section 2) of $\alpha$ in (3) with $\sigma$ known. This also induces a model-based estimate of $\lambda$ through (4), i.e.,

$\hat{\lambda}_g(\sigma) = p_g/n \cdot \sigma^2/\hat{\alpha}_g(\sigma)^2$.

In practice of course we do not know $\sigma$, nor do we necessarily believe that model (3) holds, so that $\sigma$ may not even be well-defined. Instead we treat $\sigma$ as a one-dimensional tuning parameter that may be chosen by cross-validation. The model-based procedure outlined above is then interpreted merely as a data-driven map from a one-dimensional regularization parameter $\sigma$ to a $K$-dimensional regularization vector $\lambda$. To avoid notational ambiguity, we use the typeface $\sigma$ henceforth for our tuning parameter, i.e.,

$$\sigma \mapsto \hat{\lambda}(\sigma),$$

and reserve the letter $\sigma$ only for our theoretical development as the residual noise standard deviation when model (3) is true. We then seek to choose $\hat{\sigma}$ in a model-agnostic way by cross-validation, so that $\hat{w}(\hat{\lambda}(\hat{\sigma}))$ provides close to best out-of-sample predictive performance among estimators of the family $\{\hat{w}(\hat{\lambda}(\sigma)), \sigma \in (0, \infty)\}$. We illustrate the idea in Figure 1.

\(^1\)K is fixed in our asymptotics, so that the Group Lasso may still be preferable in settings with many sparse groups.
1.2 Related work

Our theoretical contribution continues a rich line of work [Tulino and Verdú, 2004, Dicker, 2016, Dobriban and Wager, 2018, Hastie, Montanari, Rosset, and Tibshirani, 2019, Liu and Dobriban, 2019, Xu and Hsu, 2019, Dobriban and Sheng, 2020] that uses recent advances from Random Matrix Theory to precisely characterize the performance of regression methods, such as ridge or principal component regression, under high-dimensional asymptotics with dense, weak effects. Such an asymptotic perspective is relevant in application domains, e.g., genetics [Boyle et al., 2017], wherein most features are predictive of the response of interest, but the signal of each feature individually is weak. The model of dense and weak effects is to be contrasted with the traditional approach to studying high-dimensional regression through sparsity [Bühlmann and Van De Geer, 2011].

From a methodological perspective, our work is inspired by Van De Wiel, Lien, Verlaat, van Wieringen, and Wilting [2016], who introduce the Ridge regression problem with groups and provide an empirical Bayes procedure to learn the optimal penalties for logistic regression and Cox regression. However, in the case of linear regression, the approach of Van De Wiel et al. [2016] assumes that the noise level $\sigma^2$ is known or can be well-estimated from the ridge regression residuals. Instead, we provide an end-to-end estimation strategy for linear ridge regression, that furthermore is provably optimal in the high-dimensional regime.

Along the lines of Van De Wiel et al. [2016], there has been a stream of recent empirical work developing practical and reliable methods for supervised learning with feature co-data [Tai and Pan, 2007, Foo et al., 2008, Bergersen et al., 2011, Verissimo et al., 2016, Boulesteix et al., 2017, Velten and Huber, 2019, Münch et al., 2018, Perrakis et al., 2019, van de Wiel et al., 2020, Pramanik and Zhang, 2020, Tay et al., 2020, Zeng et al., 2020]. The goal of all these works is complementary and related to our paper: "co-data" is ubiquitous in modern scientific and technological applications; and so it is important to enhance the data analytic toolbox with methods that leverage side-information to improve predictive power. However, all of these previous works do not come with theoretical guarantees.\footnote{Pramanik and Zhang [2020] derive limiting risk expression for an approximate message passing (AMP) algorithm that uses side-information under the strong assumption of isotropic Gaussian covariates $x_i \sim N(0, I)$, where $I$ is the identity matrix.}

The problem of choosing multiple tuning parameters is, of course, not new. For example, when fitting generalized additive models with flexible spline expansions, one may have multiple tuning parameters to control e.g., anisotropic smoothness. The R package mgcv [Wood, 2000, 2004, 2017] provides computational routines for efficiently tuning and solving large-scale generalized additive models with many hyperparameters. mgcv is general enough, that it subsumes problem (2) and can choose tuning parameters by optimizing the GCV (generalized cross-validation) criterion, or by estimating the parameters in model (3) by restricted maximum likelihood and then using the plug-in rule (4). However, mgcv only works for $p \leq n$ and we are not aware of theoretical guarantees in high-dimensions.\footnote{It is however plausible, that the proof techniques in the present paper, along with results of Jiang, Li, Paul, Yang, and Zhao [2016] could be used to prove asymptotic optimality of mgcv. More generally, many methods have been developed to estimate the parameters in model (3) in the case of one group ($K = 1$), with the motivation of estimating heritability in genetic studies [Dicker, 2014, Dicker and Erdogdu, 2016, Janson et al., 2017, Veerman et al., 2019]. Extensions of heritability methods to $K \geq 2$ would provide alternative model-based approaches towards tuning group-regularized ridge regression.}

Finally, we note that breaking symmetry in (1) does not necessarily require introducing additional regularization parameters. The main example of an asymmetric $\text{Pen}(w)$ with a single regularization parameter is the Group Lasso penalty [Yuan and Lin, 2006],

$$
\text{Pen}_{\text{lasso}}(w) = \lambda_{\text{lasso}} \cdot \sum_{g=1}^{K} \sqrt{\frac{p_g}{p}} \left\| w_G \right\|_2.
$$

$$
(6)
$$
The group Lasso automatically selects a sparse subset of group features, i.e., most $\hat{w}_{g,i}$ are set to zero. Section 4.1 provides more details on the connection of $\sigma$-Ridge regression to the Group Lasso.

1.3 Outline

In Section 2 we elaborate on the high-level description from Section 1.1 and describe the $\sigma$-Ridge regression method in detail. In Section 3 we introduce the asymptotic framework and provide theoretical results for group-regularized ridge regression; in particular we provide a sharp expression of the limiting predictive risk when the feature covariance matrix is block-diagonal. In Section 4 we build upon the results from Section 3 and prove that $\sigma$-Ridge regression asymptotically achieves optimal prediction among all procedures of the form (2). This result holds for arbitrary feature covariance. Section 5 demonstrates promising empirical performance of $\sigma$-Ridge regression in real datasets and simulations. Finally, in Section 6 we conclude with a discussion.

2 The proposed method: $\sigma$-Ridge regression

2.1 Model based tuning with known noise variance $\sigma^2$

To motivate our proposal, let us assume that model (3) holds with known $\sigma^2$. Write $X$ for the $n \times p$ design matrix with rows $x_i^\top$ and $Y = (Y_1, \ldots, Y_n)$, $\varepsilon = (\varepsilon_1, \ldots, \varepsilon_n)$. Furthermore fix a deterministic $\tilde{\lambda}_{\text{init}} > 0$ and run ridge regression with that parameter (i.e., solve (2) with $\hat{\lambda}_{\text{init}} = (\hat{\lambda}_{\text{init}}, \ldots, \hat{\lambda}_{\text{init}})$) to get

$$\hat{w} = \left( \frac{X^\top X}{n} + \frac{\tilde{\lambda}_{\text{init}}}{n} I \right)^{-1} \frac{X^\top X}{n} w + \frac{1}{\sqrt{n}} \left( \frac{X^\top X}{n} + \frac{\tilde{\lambda}_{\text{init}}}{n} I \right)^{-1} \frac{X^\top \varepsilon}{\sqrt{n}} = M w + N \varepsilon / \sqrt{n},$$

(7)

where $I$ is the $p \times p$ identity matrix. Then under (3)

$$E \left[ \|\hat{w}_{g,\cdot}\|_2^2 \mid X \right] = \sum_{h=1}^K \|M_{g,\cdot,g_h}\|_F^2 \frac{\alpha^2}{p_h} + \|N_{g,\cdot}\|_F^2 \frac{\sigma^2}{n}, \quad g = 1, \ldots, K
$$

(8)

Here $\|\cdot\|_F$ is the Frobenius norm of a matrix, $N_{g,\cdot}$ is the matrix of the rows of $N$ corresponding to the $g$-th group and $M_{g,\cdot,g_h}$ is the $p_g \times p_h$ matrix that arises if we keep only the rows that correspond to the $g$-th group from $M$ and the columns that correspond to the $h$-th group.

Under known $\sigma$, the above system of equations directly identifies $\alpha_1, \ldots, \alpha_K$, and estimation can proceed through the method of moments. Recalling from (4) that the optimal model-based regularization parameters take the form $\lambda_g = \lambda_g(\sigma) = p_g / n \cdot \sigma^2 / \alpha^2_g$ and writing $A$ for the $K \times K$ matrix with entries $A_{gh} = \|M_{g,\cdot,g_h}\|_F^2 / n$ and $u, v$ for the vectors in $\mathbb{R}^K$ with entries $u_g = E[\|\hat{w}_{g,\cdot}\|_2^2 \mid X]$, $v_g = \|N_{g,\cdot}\|_F^2 / n$, we may rewrite the above system of equations as

$$d(\sigma) = A^{-1} \left( \frac{u}{\sigma^2} - v \right), \quad d_g(\sigma) = 1/\lambda_g(\sigma), \quad g = 1, \ldots, K$$

(9)

The data-driven method of moments estimator plugs in $\hat{u}$ with $\hat{d}_g = \|\hat{w}_{g,\cdot}\|_2^2$ in place of $u$:

$$\hat{d}(\sigma) = A^{-1} \left( \frac{\hat{u}}{\sigma^2} - v \right),$$

(10)

$^4$A data-driven choice for $\hat{\lambda}_{\text{init}}$ will be provided later.
Figure 2. **Regularization and coefficient paths in $\sigma$-Ridge regression:** The data shown here is from the same simulation as in Figure 1. **Panel a)** corresponds to panel b) of Fig. 1, with the x-axis extended to larger values of $\sigma$, and shows the map $\sigma \mapsto \hat{\lambda}(\sigma)$ from $\sigma$ to the per-group regularization parameter. Note that for large values of $\sigma$ the group-wise regularization parameter blows up to $+\infty$. **Panel b)** shows the evolution of all coefficients (2) as $\sigma$ increases. The coefficients shrink more as $\sigma$ increases, and for large enough $\sigma$, complete groups of features may be set to 0 (group-sparsity).

### 2.2 $\sigma^2$ – reinterpreting $\sigma^2$ as a regularization parameter

As we already motivated in the introduction, we may use (10) even if the model is not true, by treating the variance as a one-dimensional tuning parameter. Making this explicit by using the letter $\sigma$ instead, we let

$$
\hat{\lambda}_g(\sigma) = 1/\hat{d}_g(\sigma), \quad \text{where } \hat{d}(\sigma) = \arg\min_{d \in (0,\infty)^K} \left\{ \|Ad - \hat{u}_g\sigma^2 + v\|_2^2 \right\}
$$

(11)

The above nonnegative least squares problem can be solved in $O(K^3)$ operations. In our setting and applications, $K$ is small compared to $n, p$, so that this cost is negligible.

To provide intuition into the above we first consider the “trivial” case of one group ($K = 1$). In this case (11) takes the following form, with $\lambda(\sigma) \geq 0$:

$$
\lambda(\sigma) = \|M\|_{F}^2 / \left( \frac{n\|\hat{w}\|_2^2}{\sigma^2} - \|N\|_{F}^2 \right) +
$$

(12)

In words, $\lambda(\sigma)$ is simply a data-driven non-decreasing mapping that maps $\sigma \in [0, \infty]$ to $\lambda \in [0, \infty]$, i.e., a reparametrization. In the case of multiple groups ($K > 1$) we instead interpret $\sigma$ as yielding a regularization parameter path $\sigma \mapsto \hat{\lambda}(\sigma)$ as in (5). Figure 2 illustrates this and also shows that the path can induce group-level sparsity similar to the Group Lasso, by setting $\hat{\lambda}_g = \infty$ for some of the groups. The following proposition lists some properties of the regularization path.

**Proposition 1** (Properties of $\sigma$-regularization parameter path). Assume the matrix $A$ is invertible and $\hat{u}_g > 0$ for all $g$. Then

1. For $\sigma^2 \geq \max_g \hat{u}_g/v_g =: \sigma_{\text{max}}$, we have $\hat{\lambda}_g(\sigma) = \infty$ for all $g$, i.e. $\hat{w}\left(\hat{\lambda}(\sigma)\right) = 0$.

2. As $\sigma \to 0$, we have that $\min_g \hat{\lambda}_g(\sigma) \to 0$, i.e., at least one group is not penalized.
In light of the interpretation above, for any value of $\sigma^2$, we have a supervised algorithm that proceeds in three steps:

1. Compute $\hat{\lambda}(\sigma)$ as in (11).
2. Let $\hat{\mathbf{w}} = \hat{\mathbf{w}}\left(\hat{\lambda}(\sigma)\right)$ the Ridge regression coefficient from (2).
3. Predict the response for $x \in \mathbb{R}^p$ as $x^\top \hat{\mathbf{w}}$.

As such, we can now use any method of tuning hyperparameters to choose $\sigma$. Here we consider leave-one-out cross-validation (LOOCV). In a direct application of LOOCV, we would calculate $\hat{\lambda}^{(i)}(\sigma)$ and $\hat{\mathbf{w}}^{(i)}(\hat{\lambda}^{(i)}(\sigma))$ for each $i$, where the "$-i$" notation means that the supervised algorithm is trained based on all observations except the $i$-th. The LOOCV error is then defined as,

$$CV(\sigma) := \frac{1}{n} \sum_{i=1}^{n} \left( y_i - \hat{\mathbf{w}}^{(i)}(\hat{\lambda}^{(i)}(\sigma))^\top x_i \right)^2.$$  \hfill (13)

See Fig. 3a for a schematic of the above procedure. Finally we could choose $\sigma$ as the minimizer of $CV(\sigma)$. A downside however of this approach is that it will be computationally expensive to refit the whole model $n$ times. So instead we propose to omit the first-step of the leave-one-out procedure and keep the map $\sigma \mapsto \hat{\lambda}(\sigma)$ fixed throughout, even though it also depends on the full training set. As our prediction for observation $i$ we use $\hat{\mathbf{w}}^{(i)}(\hat{\lambda}(\sigma))^\top x_i$. We define the accelerated leave-one-out objective (also see Fig. 3b) as

$$CV^*(\sigma) := \frac{1}{n} \sum_{i=1}^{n} \left( Y_i - \hat{\mathbf{w}}^{(i)}(\hat{\lambda}(\sigma))^\top x_i \right)^2$$  \hfill (14)

3. $\mathbb{R}^+ = [0, \infty)$ may be partitioned into intervals $I_j$ in which the set $S_j = \{g : \lambda_g < \infty\}$ (i.e., the number of active groups) remains fixed. For $g \in S_j$ and $\sigma_1, \sigma_2 \in I_j$ it holds that

$$\hat{\lambda}_g(\sigma_1) = \left\{ \frac{\sigma_2^2}{\sigma_1^2} \hat{\lambda}_g(\sigma_2)^{-1} + \left( \frac{\sigma_2^2}{\sigma_1^2} - 1 \right) \hat{v}_{j,g} \right\}^{-1}, \text{ where } \hat{v}_{j,g} = \left( A_{i_g, j} A_{i_g, j}^\top \right)^{-1} A_{i_g, j} \cdot \mathbf{v}.$$

The above properties are deterministic and do not depend on the validity of (3).

### 2.3 Choosing $\sigma$ through accelerated leave-one-out cross-validation

Figure 3: Leave-one-out cross-validation (LOOCV) and accelerated LOOCV for $\sigma$-Ridge regression. The accelerated method computes the map $\sigma \mapsto \hat{\lambda}(\sigma)$ based on the full dataset and treats it as fixed when computing the leave-one-out error.

- **a) Cross-validation**
  - $\lambda^{(1)}(\sigma) \rightarrow \hat{\mathbf{w}}^{(1)}(\hat{\lambda}^{(1)}(\sigma))$
  - $\sigma \rightarrow \hat{\lambda}^{(i)}(\sigma) \rightarrow \hat{\mathbf{w}}^{(i)}(\hat{\lambda}^{(i)}(\sigma)) \rightarrow CV(\sigma)$
  - $\hat{\lambda}^{(n)}(\sigma) \rightarrow \hat{\mathbf{w}}^{(n)}(\hat{\lambda}^{(n)}(\sigma))$

- **b) Accelerated cross-validation**
  - $\sigma \rightarrow \hat{\lambda}(\sigma) \rightarrow \hat{\mathbf{w}}^{(i)}(\hat{\lambda}(\sigma)) \rightarrow CV^*(\sigma)$
The upshot is that now we may directly apply the well-known shortcut formula, cf. Meijer and Goeman [2013] and references therein. That is, letting \( \hat{\Lambda}(\sigma) \) the \( p \times p \) diagonal matrix with \( j \)-th entry equal to \( \hat{\lambda}_g(\sigma) \), when \( j \in G_g \), and

\[
H(\sigma) = X(X^\top X + \hat{\Lambda}(\sigma))^{-1}X^\top, \quad \hat{Y}(\sigma) = H(\sigma)Y,
\]

then it holds that

\[
CV^*(\sigma) = \frac{1}{n} \sum_{i=1}^n \left( Y_i - \hat{Y}_i(\sigma) \right)^2
\]

Henceforth we propose to choose \( \hat{\sigma} \) as

\[
\hat{\sigma} = \arg\min_{\sigma} CV^*(\sigma).
\]

Our theoretical analysis in Section 4 pertains to the choice of \( \sigma \) through accelerated leave-one-out cross-validation, as in (17), and demonstrates that it leads to asymptotically optimal predictions.

At this point we emphasize that the idea of using hybrid empirical Bayes/cross-validation approaches for regularization parameter tuning is not new: in the context of group-regularized ridge logistic and Cox regression, Van De Wiel et al. [2016] use empirical Bayes to learn a regularization parameter vector \( \hat{\lambda}_{GR} \) with entries \( \hat{\lambda}_{GRg} \). Then, a further ad-hoc tuning parameter \( \lambda > 0 \) is introduced, and cross-validation is used to pick a regularization vector from the family \( (\lambda \cdot \hat{\lambda}_{GR})_{\lambda > 0} \). In contrast, \( \sigma \)-Ridge, does not require knowledge of the nuisance parameter \( \sigma \) (indeed, \( \sigma/\sigma \) is the regularization parameter to be chosen by cross-validation) and we can theoretically show that it achieves optimal predictive performance (Theorem 2).

There is one missing step required to implement the full procedure; namely the choice of \( \hat{\lambda}_{init} \) in (7). Here we propose to choose \( \hat{\lambda}_{init} \) as the optimal one-dimensional ridge regression parameter, i.e., we let \( \hat{\lambda}_{init} \) be the minimizer of \( CV^*((\lambda, \ldots, \lambda)) \), where in analogy to (14), we define (with some abuse of notation):

\[
CV^*(\lambda) := \frac{1}{n} \sum_{i=1}^n \left( Y_i - \hat{w}^{-1}(i)(\lambda)^\top x_i \right)^2.
\]

Finally, we note that to solve (2), we need to factorize \( X^\top X/n + \Lambda \), where \( \Lambda \) is the diagonal matrix with \( j \)-th entry \( \lambda_g \), when \( j \in G_g \). We use the Cholesky decomposition when \( p \leq 4n \) and the Woodbury matrix identity [van Wieringen, 2020, Section 1.7] otherwise.

3 Asymptotics of group-regularized ridge regression

Before turning to study \( \sigma \)-Ridge regression, we first study the performance of group-regularized ridge regression (2) for a general choice of \( \lambda = (\lambda_1, \ldots, \lambda_K) \). The core setting for our asymptotic results is that of ridge regression with random design [Hsu et al., 2012] and random effects, that generalizes the Gaussian-Gaussian model (3):

\[
w_j \sim (0, \alpha_g^2/p_g), \quad x_i \sim F_X, \quad \varepsilon_i \sim (0, \sigma^2), \quad Y_i = x_i^\top w + \varepsilon_i
\]

Here we use the notation \( Z \sim (\mu, \tau^2) \) to denote a random variable with \( \mathbb{E}[Z] = \mu \) and \( \text{Var}[Z] = \tau^2 \). For our high-dimensional (HD) asymptotics we make the following assumptions on model (19):

(HD1) The number of groups \( K \) is fixed and \( p_g/n \to \gamma_g > 0 \) as \( n \to \infty \) for all groups \( g \). We also write \( \gamma = \sum_{g=1}^K \gamma_g \) for the asymptotic aspect ratio \( p/n \).
Let $\Sigma$ be the covariance matrix of $x_1$. There exist $h_1, h_2 > 0$ fixed such that all the eigenvalues of $\Sigma$ lie in $[h_1, h_2]$.

$x_i \sim \mathbb{P}^X$ may be written as $\Sigma^{1/2} z_i$ where $z_i \sim \mathbb{P}^Z$ has i.i.d. entries with mean zero, variance one and uniformly bounded $(8 + \eta)$-th moments for some $\eta > 0$.

The $(4 + \eta)$-th moments of $\sqrt{p} w_j$, $j = 1, \ldots, p$ and $\varepsilon_i, i = 1, \ldots, n$ are uniformly bounded.

According to (HD1), all feature groups grow at the same rate as $n, p \to \infty$. The remaining assumptions (HD2-HD4) are common for the high-dimensional analysis of ridge regression (without grouping information), see for example Dobriban and Wager [2018], Hastie et al. [2019] and Ledoit and Pêché [2011], and are typically considered to be mild. In the latter works, (HD1) is replaced by the assumption that $p/n \to \gamma > 0$ as $n \to \infty$.

They key object of our asymptotic study is the out-of-sample prediction risk of an estimator $\hat{w}$ of $w$, which we define conditionally on the training set $(X, Y)$ and true coefficient vector $w$ as

$$R(\hat{w}) = \mathbb{E} \left[ (Y_{test} - x^T_{test} \hat{w})^2 \mid X, Y, w \right]$$

where $(x_{test}, Y_{test})$ is a fresh draw from (19) (with $w$ fixed). With some abuse of notation, we also write $R(\lambda)$ for the risk of $\hat{w}(\lambda)$ from (2), i.e. $R(\lambda) = R(\hat{w}(\lambda))$.

Our first asymptotic result is that the out-of-sample prediction risk $R(\lambda)$ concentrates around its marginalization with respect to $\varepsilon, w$,

$$L(\hat{w}) = \mathbb{E} [R(\hat{w}) \mid X], \quad L(\lambda) = L(\hat{w}(\lambda)).$$

**Lemma 1.** Consider model (19) under assumptions (HD1-4). It then holds that

$$|R(\lambda) - L(\lambda)| \to 0 \ a.s.$$  

where the convergence is uniform for $\lambda$ in compact subsets of $(0, \infty)^K$. $L(\lambda)$ is equal to

$$L(\lambda) = \sigma^2 + \frac{\sigma^2}{n} \text{Tr} \left( \frac{X^T X}{n} \left( \frac{X^T X}{n} + \Lambda \right)^{-1} \Sigma \left( \frac{X^T X}{n} + \Lambda \right)^{-1} \right)$$

$$+ \frac{1}{p} \text{Tr} \left( \left( \frac{X^T X}{n} + \Lambda \right)^{-1} \Sigma \left( \frac{X^T X}{n} + \Lambda \right)^{-1} \Lambda D \Lambda \right).$$

Here, $D$ is the diagonal matrix whose $j$-th diagonal entry is $\alpha^2 g_j/p_g$, when $j \in G_g$.

The proof relies on an application of the Marcinkiewicz-Zygmund interpolation [Erdos and Yau, 2017, Chapter 7] leveraging the boundedness of the $(4 + \eta)$-th moments of $w_j$ and $\varepsilon_i$. The upshot of Lemma 1 is that the only source of randomness in $L(\lambda)$ is through trace functionals of the sample covariance matrix $X^T X/n$, which can be characterized precisely using techniques from Random Matrix Theory [Yao, Zheng, and Bai, 2015].

### 3.1 Sharp risk predictions under block-diagonal covariance

As a first application of Lemma 1, we seek to provide exact and deterministic expressions for the limiting predictive risk $R(\lambda)$ of group-regularized ridge regression for any choice of $\lambda \in (0, \infty)^K$. Such results have previously been derived in the setting without groups ($K = 1$) [Dicker, 2016, Dobriban and Wager, 2018, Hastie, Montanari, Rosset, and Tibshirani, 2019]. The key assumption in these works is that the empirical distribution of the eigenvalues of the feature covariance matrix $\Sigma$ converges to a limiting spectral distribution $H$; the limiting risk formulae then are functions of only $H$, the regularization parameter $\lambda > 0$ and the asymptotic aspect ratio $\gamma = \lim_{n \to \infty} p/n$. In the setting with groups, we assume that such convergence holds within each subgroup and assume in addition to (HD1-4) that
Each group of features \( g \in \{1, \ldots, K \} \) has a covariance matrix \( \Sigma_g \) with limiting spectral distribution \( H_g \) as \( n \to \infty \).

In the grouped setting, in contrast to the setting without groups, assumption (A1) does not suffice (as we explain below). We thus also assume that:

(A2) We assume that predictors are uncorrelated across groups, i.e., we impose a block diagonal structure on \( \Sigma \).

\[
\Sigma = \begin{pmatrix}
\Sigma_1 & 0 & \cdots & 0 \\
0 & \Sigma_2 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & \Sigma_K 
\end{pmatrix}
\]

We also allow finite rank perturbations of such block diagonal matrices.

Assumption (A2) is strong. However, an assumption of such kind is necessary. Otherwise the predictive risk may not converge to an asymptotic limit. Furthermore, even when the asymptotic limit exists, the limiting expression will typically not be a function of only the group-wise spectral distributions \( H_1, \ldots, H_K \). For example, if the eigenvectors of \( \Sigma \) are sufficiently delocalized (such as uniformly distributed with respect to the Haar measure), then the limit that arises is going to be different than the limit arising from the Block-Diagonal structure in (A2) with the same \( H_1, \ldots, H_K \).

Among assumptions under which the predictive risk converges to a limit, we consider Assumption (A2) to provide a realistic approximation for some practical settings. For instance, factor models in finance as in Ait-Sahalia and Xiu [2017], Tao et al. [2017] assume that financial returns lie close to a low dimensional space of principal components and that the residuals tend to have a block-diagonal covariance structure with each block corresponding to a different market sector.

The key result of this section is the following Theorem:

**Theorem 1** (Asymptotic risk of group-regularized ridge regression). Consider model (19) under assumptions (HD1-4), (A1-2) and also assume that \( x_i \sim N(0, \Sigma) \) and \( \sigma^2 = \text{Var}[\varepsilon_i] = 1 \).

We perform group-regularized ridge regression (2) with deterministic parameters \( \lambda = (\lambda_1, \ldots, \lambda_K) \in (0, \infty)^K \) to estimate \( w \). The out-of-sample regression risk \( R(\lambda) = R(\hat{w}(\lambda)) \) converges almost surely to

\[
1 + \gamma f(\lambda_1, \cdots, \lambda_K) + \sum_{j=1}^K \frac{\gamma_j}{\gamma} (\gamma_j \lambda_j - \alpha_j^2 \lambda_j^2) \frac{\partial f(\lambda_1, \cdots, \lambda_K)}{\partial \lambda_j},
\]

where \( f = f(\lambda_1, \cdots, \lambda_K) \geq 0 \) is the unique solution of the equation

\[
f = \sum_{j=1}^K \frac{\gamma_j}{\gamma} \int \left( \frac{\lambda_j}{t} + \frac{1}{1 + \gamma f} \right)^{-1} dH_j(t).
\]

We emphasize that the limiting risk formula of Theorem 1 only depends on the group-wise spectra \( H_1, \ldots, H_K \), the limiting aspect ratios \( \gamma_1, \ldots, \gamma_K \) and the regularization parameters \( \lambda_1, \ldots, \lambda_K \) and so the result directly generalizes existing results in the case \( K = 1 \) [Dicker, 2016, Dobriban and Wager, 2018, Hastie, Montanari, Rosset, and Tibshirani, 2019]. The extension to the grouped

\textit{5}Our proof techniques can be used to derive limiting expressions in such situations too, but we do not carry out this analysis here.

\textit{6}These two additional assumptions are not important. The assumption \( \sigma^2 = 1 \) is merely aesthetic and simplifies the formulae. The assumption \( x_i \sim N(0, \Sigma) \) simplifies our technical arguments and could be replaced by assumption (HD3).
setting leads to technical complications; the arguments of aforementioned papers rely on symmetry properties (say, invariance with respect to rotations) which no longer hold in the presence of grouping information.

We now give an example of how to apply Theorem 1: Consider the case $K = 2$ with two groups with aspect ratios $\gamma_1, \gamma_2$ and point mass spectra $H_1 = H_2 = \delta_1$ (i.e., $\Sigma = I$). We then need to solve (for $f \geq 0$) the equation

$$f = \frac{\gamma_1}{\gamma} \left( \lambda_1 + \frac{1}{1 + \gamma f} \right)^{-1} + \frac{\gamma_2}{\gamma} \left( \lambda_2 + \frac{1}{1 + \gamma f} \right)^{-1},$$

which is equivalent to a cubic equation in $f$ of which we pick the unique non-negative root. To get the asymptotic risk, we would then plug-in $f$ to formula (22), which also depends on the group-wise signal strengths $\alpha_1, \alpha_2$. Supplement C.3 studies equation (23) more generally and explains how to solve it numerically.

As a first corollary of Theorem 1, we compute the optimal predictive risk attainable by group-regularized ridge regression.

**Corollary 1.** Under the assumptions of Theorem 1, the (asymptotically) optimal choice of regularization parameters is given by $\lambda_g^* = \gamma_g/\alpha_g^2$ (i.e., (4) with $p_g/n$ replaced by its limit). The optimal limiting risk is equal to $1 + \gamma f(\lambda_1^*, \ldots, \lambda_K^*)$ with $f$ given by (23).

### 3.2 Using a single regularization parameter

Theorem 1 enables us to theoretically answer and provide quantitative insights into questions as follows. Consider two groups of features, i.e., $K = 2$. Analyst 1 has access only to features $X_{G_1}$ and optimally tunes ridge regression. Analyst 2 also has access to the second set of features, i.e., to both $X_{G_1}$ and $X_{G_2}$. Analyst 2, however, is not aware of the grouping and runs ridge regression with a single (optimal) regularization parameter. When is Analyst 1 better off than Analyst 2? This tradeoff, will depend on the size of $G_2$ and the strength of its signal. Intuitively, if the signal in $G_2$ is low, then Analyst 1 is better off, since the additional set of features swamps the regression of Analyst 2 with noise. On the other hand, if signal is strong, then Analyst 1 misses out on informative features.

Our first result is the following, which describes the asymptotically optimal parameter when the limiting spectral distributions are the same for the covariance matrices of each group.

**Corollary 2.** Consider the case of $K$ groups such that $H_g = H_{g'}$ for all groups $g, g'$. Then, the optimal choice of a single regularization parameter is asymptotically equal to

$$\lambda^* = \frac{\gamma}{\sum_{g=1}^K \alpha_g^2}.$$

If $H_1, \ldots, H_K$, were not all the same, then the above statement would no longer be true, since groups with higher predictor variability would affect $\lambda^*$ in different proportions.

---

7While we were finishing this work, we became aware of parallel work by Wu and Xu [2020] who derive asymptotic risk predictions for ridge regression with general quadratic penalties that subsume the diagonal, group-wise constant penalty matrices that we consider. When specialized to our setting, their asymptotic risk formulae are less natural than ours as they are not phrased in terms of $\lambda_1, \ldots, \lambda_K$, but instead in terms of a single penalty parameter, say $\lambda_1$, and a function $h$ that depends on the value of the ratios $\lambda_2/\lambda_1, \ldots, \lambda_K/\lambda_1$ in an implicit way. Furthermore, Wu and Xu [2020] do not address the key issue of data-driven choice of the optimal regularization parameters.

8If both analysts tune their methods suboptimally, say with a very small regularization parameter value, then Analyst 2 may have an advantage due to the implicit regularization of noise features, cf. the double descent phenomenon described for Ridge regression by Hastie, Montanari, Rosset, and Tibshirani [2019]. Our results also enable the study of this phenomenon.
For the rest of this section we assume that $\Sigma = I$ so as to provide more explicit formulae. Our next corollary explains how introducing an unimportant group of features can hurt predictive performance of ridge regression.

**Corollary 3.** The prediction risk for $\lambda = (\lambda, \ldots, \lambda)$ and $\Sigma = I$ converges almost surely to

$$\frac{1}{u} - \frac{\gamma \lambda - (\sum_{y=1}^{K} \tilde{\alpha}_y^2) \lambda^2}{(\lambda + u)^2 - \gamma u^2}, \text{ where } u = \frac{1 - \gamma - \lambda + \sqrt{(\lambda + \gamma - 1)^2 + 4\lambda}}{2}.$$

The optimal asymptotic risk in this case is given by

$$\gamma + \lambda^* - 1 + \frac{(\gamma + \lambda^* - 1)^2 + 4\lambda^*}{2\lambda^*},$$

with $\lambda^*$ as in (24). In particular, for the case of 2 groups ($K = 2$) and $\Sigma = I$, where only the first group is important for prediction, that is $\alpha_2 = 0$, the optimal prediction risk for ridge regression with a single prediction parameter is asymptotically equal to

$$\gamma + \frac{\gamma_2}{\alpha_2^2} + \left(\frac{\gamma + \frac{\gamma_2}{\alpha_2^2} - 1}{\alpha_2^2}\right) + 4\frac{\gamma_2}{\alpha_2^4}.$$

The last expression is increasing in $\gamma_2$ (holding $\gamma_1$ fixed) and converges to $1 + \alpha_1^2$ as $\gamma_2 \to \infty$.

The existence of unimportant features, as expected, hurts the performance of optimally-tuned ridge regression with a single regularization parameter. We next proceed to answer the motivating question asked in the beginning of this section, i.e., the case $K = 2$ with two analysts, wherein Analyst 1 has access only to the first feature group, while Analyst 2 has access to both but is not aware of the grouping information.

**Corollary 4.** If we ignore the second group of predictor variables, the optimal ridge regression prediction risk is

$$(\alpha_2^2 + 1)\frac{\gamma_1 + \lambda - 1 + \sqrt{(\gamma_1 + \lambda - 1)^2 + 4\lambda}}{2\lambda}, \text{ with } \lambda = \frac{\gamma_1(\alpha_2^2 + 1)}{\alpha_1^2}.$$ 

Thus, if we use a single regularization parameter, performance is hurt by the presence of the second group, if (for $\lambda^* = \gamma/(\alpha_1^2 + \alpha_2^2)$) it holds that

$$\frac{\gamma + \lambda^* - 1 + \sqrt{(\gamma + \lambda^* - 1)^2 + 4\lambda^*}}{2\lambda^*} \geq (\alpha_2^2 + 1)\frac{\gamma_1 + \lambda - 1 + \sqrt{(\gamma_1 + \lambda - 1)^2 + 4\lambda}}{2\lambda}. \quad (25)$$

Corollary 4 allows us to find for any fixed choices of $\alpha_1, \gamma_1, \gamma_2$ the threshold below which $\alpha_2$ makes the presence of the second group harmful. Some example consequences, are as follows. Consider the regime of a very strong signal in group 1 ($\alpha_1 \to \infty$), then

- If $\gamma < 1$ and $\alpha_2^2/\gamma_2 > 1/(1 - \gamma)$, then the presence of the second group improves the prediction risk for any value of $\gamma_1$. The LHS in this condition corresponds to the “signal-to-noise” ratio in group 2, while the RHS is equal to the out-of-sample risk of unregularized linear regression.
- If $\gamma > 1$, then including the second group of predictor variables and using a single regularization parameter hurts predictive performance.
triangles correspond to the finite-sample risk evaluated by simulations. The aspect ratios \( \gamma_1, \gamma_2 \) and signal strengths \( K_1, K_2 \) are the same for all panels of Figure 4, while the relative signal strength in the first group \((\alpha_1^2/(\alpha_1^2 + \alpha_2^2))\) varies along the \( x \)-axis of the panels.

### 3.3 Numerical illustration of asymptotic risk predictions

In this subsection we illustrate the theoretical risk curves derived in Theorem 1. We consider the case \( K = 2, n = 1000 \) and \( \Sigma = I \) and show risk curves as a function of \( \gamma_1, \gamma_2 \) and the signal strengths \( \alpha_1^2, \alpha_2^2 \) with \( \lambda \) chosen in the following 3 ways: 1) \( \lambda \) is the optimal regularization parameter vector defined in (4), 2) \( \lambda \) is the optimal regularization parameter among parameters of the form \( \lambda = (\lambda, \lambda) \) (i.e., we use both features but use a single regularization parameter) and 3) the optimal parameter among parameters of the form \( \lambda = (\lambda, \infty) \), (i.e., we omit the second group of features).

Figure 4 shows the theoretical curves from (4) along with an empirical estimate of the test error of the method (computed by generating 20,000 test samples and computing the error on these) based on a single realization of the simulation; i.e., the triangles correspond to \( R(\lambda) \) (20). We observe the excellent agreement between theoretical and finite-sample results. As expected, in all panels of Figure 4, we observe that group-regularized ridge regression decreases prediction risk the most under strong heterogeneity across groups \( \alpha_1 \neq \alpha_2 \). When \( \alpha_2 \approx 0 \), ridge regression on the first group of features has about the same risk as group-regularized ridge regression. The exact details of the risk curves depend on the corresponding data generating mechanism (through the spectra \( H_1, H_2 \), aspect ratios \( \gamma_1, \gamma_2 \) and signal strengths \( \alpha_1, \alpha_2 \)). In supplementary Figure S1 we demonstrate risk curves under a more complicated covariance structure (following Dobriban and Wager [2018]); we let \( \Sigma_1 = \Sigma_2 \), each with eigenvalues corresponding to evenly-spaced quantiles of the Exponential distribution with rate 0.5. The conclusions are similar.
4 High-dimensional optimality of σ-Ridge Regression

Our main result in this section is the asymptotic optimality of σ-Ridge regression under model (19). Concretely, we show that, asymptotically, σ-Ridge regression matches the prediction risk of the best possible predictor from the class (2). Our Theorem builds upon the asymptotic setting from Section 3.

**Theorem 2 (Optimality of σ-Ridge Regression).** Consider model (19) under assumptions (HD1-4). Let \( V_1 \subset (0, \infty) \) a compact set with \( \sigma \in V_1 \) and \( V_2 \) a subset of \((0, \infty)^K\) bounded away from 0. We choose \( \hat{\sigma} = \arg\min_{V_1} CV^* (\sigma) \). Then:

\[
\limsup_{n \to \infty} \left( R(\hat{\lambda}) - \inf_{\lambda \in V_2} R(\lambda) \right) \leq 0 \text{ a.s.}
\]

This result is true for any (potentially data-driven) choice of \( \lambda_{init} \in V_3 \) in (7), where \( V_3 \subset (0, \infty) \) is also a compact set.

For example, under the conditions of Theorem 2, in particular when \( \Sigma \) is block-diagonal, the above Theorem implies that the asymptotic risk of σ-Ridge is equal to the expression in Corollary 1. However, we emphasize that the result of Theorem 2 is applicable to any feature covariance matrix \( \Sigma \) (as long as all the eigenvalues of \( \Sigma \) remain bounded away from 0 and \( \infty \)).

Before proceeding with the proof of Theorem 2, we first apply it to elucidate the connection of σ-Ridge regression and the Group Lasso [Yuan and Lin, 2006].

4.1 σ-Ridge regression and the Group Lasso

As already mentioned in Section 1.2, the Group Lasso is a regularized regression method as in (1) that penalizes the Euclidean Norm of group-wise coefficients (6), i.e.,

\[
\hat{\mathbf{w}}_{\text{glasso}} = \inf_{\mathbf{w}} \left\{ \frac{1}{2n} \sum_{i=1}^{n} (Y_i - x_i^\top \mathbf{w})^2 + \lambda_{\text{lasso}} \sum_{g=1}^{K} \frac{p_g}{p} \| \mathbf{w}_{G_g} \|_2 \right\}
\]

A beautiful aspect of the Group Lasso is that it enforces group-wise sparsity, i.e., for many groups it holds that \( \hat{\mathbf{w}}_{\text{lasso}}^{G_g} = 0 \) and it has strong recovery guarantees of the non-zero groups (similar to the Lasso in the setting without groups). At first sight, the Group Lasso method (26) and group-regularized ridge regression (2) may seem unrelated. However, it turns out that (2) can recover (26) by appropriate choice of \( \lambda \): if we set the components of \( \lambda \) as \( \lambda_g = \lambda_{\text{lasso}} \cdot \sqrt{\frac{p_g}{p}} \| \hat{\mathbf{w}}_{\text{lasso}}^{G_g} \|_2 \) (with the convention that \( \lambda_i = \infty \) if the denominator is 0), then

\[
\hat{\mathbf{w}}(\lambda) = \hat{\mathbf{w}}_{\text{lasso}}(\lambda_{\text{lasso}})
\]

The intuition behind this result is that we can write \( \| \mathbf{w}_{G_g} \|_2 = \| \hat{\mathbf{w}}_{\text{lasso}}^{G_g} \|_2^2 / \| \hat{\mathbf{w}}_{\text{lasso}}^{G_g} \|_2 \): a formal verification proceeds by checking the Karush-Kuhn-Tucker conditions. In other words, we may also think of the Group-Lasso as providing a map from 1D regularization parameter \( \lambda_{\text{lasso}} \) to the \( K \)-dimensional \( \lambda \), that is then used along with the group-regularized ridge objective (2). The construction of the path is motivated by sparsity considerations, while the σ-Ridge path is motivated by models (3) and (19). A consequence of (27) and Theorem 2, is the following result:

\footnote{The results here were motivated by Section 6 of Tay, Aghaeepour, Hastie, and Tibshirani [2020].}

\footnote{We note, that σ-Ridge regression can also select groups of features (cf. Figure 2). Our focus on this paper, however, is on predictive performance.}
Corollary 5 ($\sigma$-Ridge regression is at least as powerful as the Group Lasso). Under the assumptions of Theorem 2 and for any fixed $\delta > 0$, it holds that

$$\limsup_{n \to \infty} \left( R(\hat{w}(\hat{\lambda})) - \inf_{\lambda_{\text{glasso}} \geq \delta} R(\hat{w}_{\text{glasso}}(\lambda_{\text{glasso}})) \right) \leq 0 \text{ a.s.}$$

In interpreting this result, we caution, however, that the Group Lasso has been developed in the context of group-wise selection of features, when most feature groups are assumed to have no signal and the number of groups is potentially large. Consequently, the setting of Corollary 5 favors $\sigma$-Ridge regression. Nevertheless, the result does provide some guidance to practitioners about the types of datasets in which $\sigma$-Ridge regression would be preferable over the Group Lasso. We return to this comparison, from an empirical perspective, in Section 5.

4.2 Intermediate results leading to the proof of Theorem 2

The proof of Theorem 2 hinges on Lemma 1, as well as two additional Lemmata that are of independent interest, and that we now describe.

Our first lemma justifies the use of the method of moments in (8).

Lemma 2. Under the assumptions of Theorem 2 we have for each $g = 1, \cdots, K$:

$$\|\hat{w}_g\|_2^2 - \left( \sum_{h=1}^K \|M_{g_g} v_h\|_F^2 \frac{\alpha_h^2}{p_h} + \|N_{g_g} \|^2_F \frac{\sigma^2}{n} \right) \xrightarrow{a.s.} 0. \tag{28}$$

In addition, the matrix $A$ in (11) (cf. system (8)) is invertible almost surely for all large $n$ and the inverse has bounded operator norm. It follows that, if we solve (11) at $\sigma = \sigma$, then:

$$\hat{\lambda}_g(\sigma) - \frac{p_g}{n} \frac{\sigma^2}{\sigma_g^2} \to 0 \text{ a.s.} \tag{29}$$

The first result, i.e., (28), follows very similarly to the proof of Lemma 1 and uses Marcinkiewicz-Zygmund interpolation along with the uniform moments bounds we have assumed. The second result, i.e., the study of the matrix $A$, is more technically challenging. In the process of our proof (in Supplement D), we develop techniques for lower bounding the eigenvalues of a matrix that is formed by taking a larger symmetric matrix, squaring its entries and then summing the squares in a block-wise fashion.

Our second Lemma shows that the leave-one-out objective $CV^*(\lambda)$ from (18) is uniformly close to $L(\lambda)$.

Lemma 3. Under the assumptions of Theorem 2 we have

$$|CV^*(\lambda) - L(\lambda)| \to 0 \text{ almost surely as } n \to \infty,$$

uniformly for $\lambda$ in compact subsets of $(0, \infty)^K$.

Along with Lemma 1, it follows that the leave-one-out estimate of the error is close to the true out-of-sample error. Similar results in the case of a single regularization parameter (e.g., ridge regression with a single group) have a long tradition in the statistics literature, see for example [Li, 1987]. More recently, such results have resurfaced under the lens of high-dimensional asymptotics and random matrix theoretic results. For example, in the setting without side-information, Xu et al. [2019] study leave-one-out cross-validation for many penalties, but with restrictive assumptions on the distribution of the features $x_i$. Hastie, Montanari, Rosset, and Tibshirani [2019] prove a result analogous to Lemma 3 in the case of a single group (i.e., without side information) and for
feature covariance $\Sigma$ with a limiting spectral distributions. Their proof relies on the fact that the two estimates of the risk have explicit formulas. In the case of group-regularized ridge regression and without assumptions of convergence of the spectral distribution of the population covariance matrix, such explicit formulas are not available, and so the proof (in Supplement D) is more involved.

With the three key Lemmata 1, 2 and 3 in hand, we are ready to prove Theorem 2.

4.3 Proof of Theorem 2

Proof. We assume that $V_2$ is a fixed compact set; and provide the extension to noncompact $V_2$ in the supplement. Since $L(\lambda) - R(\lambda) \to 0$ uniformly over $V_2$ by Lemma 1, it follows that

$$\inf_{V_2} L(\lambda) - \inf_{V_2} R(\lambda) \xrightarrow{a.s.} 0.$$ 

Since the formula for $L(\lambda)$ is universal among all distributions on $w_j, \varepsilon_i$ with the moment assumptions that we made, it is, in particular, the expected risk for a model with Gaussian priors on the coefficients and Gaussian errors. In that case, the optimal coefficient vector corresponds to the posterior mean, which is achieved for $\lambda^* = (\sigma^2 p_g n^{-1} \alpha_g^{-2})_{1 \leq g \leq K}$, cf. (4). We conclude that this choice minimizes $L(\lambda)$, and so

$$\lim_{n \to \infty} \sup \left( L(\lambda^*) - \inf_{V_2} R(\lambda) \right) \leq 0 \text{ a.s.}$$

It thus suffices to show that

$$\lim_{n \to \infty} \sup \left( R(\hat{\lambda}(\hat{\sigma})) - L(\lambda^*) \right) \leq 0 \text{ a.s.}$$

One can verify that the functions $L$ are almost surely equicontinuous at $\lambda^*$. By Lemma 2, we get for $\sigma = \sigma$ that $\lambda(\sigma) - \lambda^* \to 0$ almost surely and consequently also $L(\lambda(\sigma)) - L(\lambda^*) \xrightarrow{a.s.} 0$. It remains to show that

$$\lim_{n \to \infty} \sup \left( R(\hat{\lambda}(\hat{\sigma})) - L(\lambda(\sigma)) \right) \leq 0 \text{ a.s.}$$

By Lemma 1, Lemma 3 and the definition of $\hat{\sigma}$ we conclude that indeed almost surely

$$R(\hat{\lambda}(\hat{\sigma})) - L(\lambda(\sigma)) = CV^* (\hat{\lambda}(\hat{\sigma})) - CV^* (\lambda(\sigma)) + o(1) \leq o(1).$$

5 Numerical results

In this section we show that $\sigma$-Ridge regression is practical. To this end, in Subsections 5.1, 5.2, we apply $\sigma$-Ridge regression to real datasets from two distinct domains and show its low out-of-sample prediction error. In these datasets, model (19) is unlikely to hold, and so our theoretical results are not applicable, but nevertheless $\sigma$-Ridge regression performs favourably. In Subsection 5.3 we conduct a simulation study when the data-generating mechanism is indeed specified by model (19).

Throughout this section, we compare the following four methods.

1. $\sigma$-Ridge, i.e., the regression method introduced in this work, tuned via accelerated leave-one-out cross-validation (14). $\sigma$ is chosen from an equidistant grid of 100 points between $10^{-3} \cdot \sigma_{\text{max}}$ to $\sigma_{\text{max}}$, where $\sigma_{\text{max}}$ is defined in the first part of Proposition 1.

\footnote{Equality would be attained if $V_2$ is such that $\lambda^* \in V_2$.}
2. **Single Ridge**, i.e., Ridge regression with a single regularization parameter $\lambda$ (the same across all feature groups), tuned via leave-one-out-cross validation (LOOCV) (18). We choose $\lambda \in L_{\text{grid}}$, where $L_{\text{grid}}$ is a logarithmically equidistant grid of 100 points from $10^{-6} \cdot \lambda_{\max}$ to $\lambda_{\max}$, where $\lambda_{\max}$ is chosen equal to $10^4 \cdot \|X^\top Y/n\|_{\infty}$ (the default choice of $\lambda_{\max}$ in the glmnet package [Friedman et al., 2010])

3. **Multi Ridge**, i.e. Group Ridge regression (2) with one regularization parameter per group, tuned via LOOCV (18). $\lambda \in (0, \infty)^K$ is chosen from 1000 randomly selected points from the product grid $L_{\text{grid}}^K$, where $L_{\text{grid}}$ is the grid used for Single Ridge regression.

4. **Group Lasso** [Yuan and Lin, 2006], as in (26). Here the shortcut-trick for LOOCV is not applicable, so we tune $\lambda^{\text{gl}} = \lambda^{\text{lasso}}$ by monitoring the mean squared error on a holdout set with 30\% of the observations. $\lambda^{\text{gl}}$ is chosen from a logarithmically equidistant grid that ranges from $10^{-5} \cdot \lambda_{\max}^{\text{grid}}$ to $\lambda_{\max}$, where $\lambda_{\max}^{\text{grid}} = n^{-1} \max_g \{ \|(X^\top Y)_g\|_{\infty}/\sqrt{p_g/p} \}$, i.e., the smallest $\lambda^{\text{gl}}$ so that $g^{\text{lasso}}(\lambda^{\text{gl}}) = 0$.

5.1 Drug response in chronic lymphocytic leukemia

Our first dataset comes from high-throughput biology. Dietrich et al. [2018] collected data from different blood cancer patients on the ex-vivo viability of cells after exposure to different drugs, as well as molecular profiling data with measurements of RNA-Seq expression and DNA methylation. The response of interest $Y_i$ is the ex-vivo viability of the cells of patient $i$ after treatment with Ibrutinib (a drug used to treat chronic lymphocytic leukemia). There are $n = 121$ patient samples with $p = 9553$ features that may be partitioned into three groups: $G_{\text{Drugs}}$, the response (ex-vivo viability) to 61 drugs (different from Ibrutinib) measured at 5 different concentrations ($p_{\text{Drugs}} = 305$), and $G_{\text{Methyl}}, G_{\text{RNA}}$ corresponding to the $p_{\text{Methyl}} = 4248$, $p_{\text{RNA}} = 5000$ most variable methylation, resp. RNA-Seq expression measurements. We refer to Dietrich et al. [2018] for more details, as well as Velten and Huber [2019], Pramanik and Zhang [2020] for further analyses of this dataset.

| Method          | Tuning | $\hat{\lambda}_{\text{Drugs}}$ | $\hat{\lambda}_{\text{Methyl}}$ | $\hat{\lambda}_{\text{RNA}}$ | Time (s) | RMSE   |
|-----------------|--------|------------------------|------------------------|------------------------|----------|--------|
| Single Ridge    | $\hat{\sigma} = 0.00197$ | 1.47e-5 | Inf | Inf | 7.30 | 0.0510 |
| Multi Ridge     | 0.00082 | 0.00082 | 0.00082 | 8.76 | 0.0785 |
| Group Lasso     | $\hat{\lambda}^{\text{gl}} = 0.147$ | 0.133 | 2.75 | 10.9 | 94.3 | 0.0511 |

Table 1: **Results on chronic lymphocytic leukemia dataset**: We report data-driven tuning parameters selected by each method, as well as the implied choice of $\hat{\lambda} = (\hat{\lambda}_{\text{Drugs}}, \hat{\lambda}_{\text{Methyl}}, \hat{\lambda}_{\text{RNA}})$. We note that Single/Multi Ridge directly tune $\lambda$. We also report the time required for running the whole procedure and the RMSE (root mean squared error) estimated by 10-fold cross-validation.

After standardizing the response and the features (to sample mean 0 and sample variance 1), we apply the four different regression methods on the full dataset ($n = 121$). The results are shown in Table (1), where we show the data-driven choice of tuning parameters and the implied values of $\hat{\lambda}$ (for the Group Lasso we define $\hat{\lambda}$ as in (27)). We also report the time it takes to fit the full regression models\textsuperscript{12}, including the time required for data-driven tuning. Furthermore, we split the dataset into 10-folds, and then use cross-validation to evaluate the root mean squared error (RMSE) of the four methods. In terms of RMSE, $\sigma$-Ridge and the Group Lasso perform best.

\textsuperscript{12}Algorithm run-times were evaluated on a single core of a Macbook Pro with a 2.6 GHz 6-Core Intel Core i7 processor and capture the whole (accelerated) leave-one-out procedure. The goal of the timings is to demonstrate that $\sigma$-Ridge regression is practical. Precise timings for all these methods will vary substantially depending on computing device and algorithmic/implementation choices (matrix decompositions used, convex optimization routines, numerical tolerances and so forth).
Both only mildly regularize $G_{\text{Drugs}}$, while regularization for $G_{\text{Methyl}}, G_{\text{RNA}}$ is more aggressive; in fact $\sigma$-Ridge regression completely discards these groups by setting $\hat{\lambda}_g = \infty$. This makes sense from a biological perspective: the drug measurements of ex-vivo viability are phenotypically close to the response of interest, i.e., the ex-vivo viability to another drug (Ibrutinib). In contrast, Single Ridge and Multi Ridge apply mild regularization to the latter groups, and their error is larger.

| Tuning  | $\hat{\lambda}_{\text{Drugs}}$ | $\hat{\lambda}_{\text{Methyl}}$ | $\hat{\lambda}_{\text{RNA}}$ | $\hat{\lambda}_{\text{Noise}_1}$ | $\hat{\lambda}_{\text{Noise}_2}$ | Time (s) | RMSE   |
|---------|-------------------------------|-------------------------------|-------------------------------|---------------------------------|----------------------------------|----------|--------|
| $\sigma$-Ridge | 1.52e-5                       | Inf                           | Inf                           | Inf                             | Inf                              | 8.110    | 0.0510 |
| Single Ridge | 0.00082                       | 0.00082                       | 0.00082                       | 0.00082                         | 0.00082                          | 6.94     | 0.0799 |
| Multi Ridge | 0.00082                       | 0.00218                       | 0.00125                       | 0.00331                         | 154.0                            | 64.9     | 0.0985 |
| Group Lasso | $\hat{\lambda}_{\text{gl}} = 0.106$ | 0.0953                       | 2.31                          | 8.42                            | 2.08                             | 170.0    | 0.0521 |

Table 2: Results on chronic lymphocytic leukemia dataset: This Table is analogous to Table 1; the main difference is that we repeat the analysis of the dataset after adding two additional groups of features that correspond to noise.

We then repeat the same evaluation after adding two groups of noise features to $X$. The first noise group consists of permuted drug measurements ($p_{\text{Noise}_1} = 305$), while the second noise group consists of $p_{\text{Noise}_2} = 100$ i.i.d. Standard Gaussian measurements that are independent of everything else. Results are shown in Table 2 and are qualitatively similar to the results from Table 1. $\sigma$-Ridge automatically discards the two noise groups as well, by setting their $\hat{\lambda}_g = \infty$.

### 5.2 Release year in the one million songs dataset

As our second empirical example, we seek to predict the release year of different songs based on ‘timbre’ features. The dataset we use is a subset of the Million Song Dataset [Bertin-Mahieux et al., 2011] that is made available through the UCI Machine Learning repository [Dua and Graff, 2020]. We refer the reader to Dobriban and Sheng [2020] for another analysis of this dataset using distributed ridge regression that does not account for the group structure of the features.

The dataset consists of $n = 515,345$ samples and it has already been split into training (463,715) and test subsets (51,630 samples). Each sample $i$ corresponds to a song: the response $Y_i$ is the year of release. The raw data for each song consists of segments and 12 timbre attributes per segment. These are converted into features $x_i \in \mathbb{R}^{156}$ as follows: First, each timbre attribute is averaged across all song segments; this yields a group of 12 features $G_{\text{mean}}$. The next 12 features $G_{\text{std}}$ are computed as the standard deviation of the raw timbre attributes. The features in $G_{\text{cov}}$ consist of the $66 = \binom{12}{2}$ pairwise covariances of the raw timbre attributes, and similarly $G_{\text{corr}}$ of the 66 pairwise correlations. In total we thus have $K = 4$ groups of features with $p_1 = p_2 = 12$ and $p_3 = p_4 = 66$.

For $n \in \{200, 1000, 5000\}$ and 20 Monte Carlo replications, we randomly subsample the training set to $n$ so as to increase the difficulty of the prediction task. We then standardize (to sample mean 0 and sample variance 1) the response and features and apply the 4 regression methods with data-driven tuning. The mean squared error is evaluated based on all the test samples. Figure 5 shows the mean squared error (MSE) and time required to apply each regression method for each Monte Carlo replicate and each subsample size. We observe that $\sigma$-Ridge Regression outperforms the other methods in terms of MSE and has running time comparable to Single Ridge. Multi Ridge tuned by cross-validation has comparable MSE but is slower. The advantage of $\sigma$-Ridge regression is most pronounced for small sample sizes ($n \in \{200, 1000\}$), while all methods perform well for $n = 5000$.

In Figure 6 we show the data-driven regularization parameters $\hat{\lambda}$ assigned by each of the four methods (for each training subsample) to the four feature groups. We first discuss the regularization
Figure 5: Empirical comparison using the One Million Song dataset [Bertin-Mahieux et al., 2011]: We compare four methods on subsamples of the full dataset; each column corresponds to a different subsample size. We repeat the subsampling 20 times. Each point corresponds to a combination of subsample and regression method. In (a) we show the mean squared error evaluated on a larger test set, while in (b) we compare the timing.
a) $n = 200$

![Graphs for $n = 200$](image)

b) $n = 1000$

![Graphs for $n = 1000$](image)

c) $n = 5000$

![Graphs for $n = 5000$](image)

Figure 6: Data-driven penalization in the One Million Song dataset [Bertin-Mahieux et al., 2011]: This is a companion figure to Figure 5. The rows correspond to the columns of Fig. 5. The columns here correspond to the $K = 4$ different feature groups and each panel shows the $\hat{\lambda}_g$ applied by each method to each feature group and for each subsample.

parameters learned by $\sigma$-Ridge regression. We observe that across all subsamples, $\hat{\lambda}_\text{mean}$ is almost 0; and so the feature group $G_\text{mean}$ appears to be important for prediction. $\hat{\lambda}_\text{std}$ on the other hand varies across subsample runs. It is typically larger for smaller training sets: the smaller $n$ is, the stronger the regularization. A similar trend is observed for $G_\text{cov}$, while the features in $G_\text{cor}$ appear to be less important, so that penalization is occasionally strong even for $n = 5000$. The trend for the data-driven choices of $\hat{\lambda}$ is also similar for Multi Ridge and Group-Lasso (although the Group-Lasso performs worse in terms of MSE). Single Ridge struggles at $n \in \{200, 1000\}$ as it is forced to penalize the informative features $G_\text{mean}$ so as to control overfitting on features in the other groups. In contrast, all other methods, leverage the side-information on the features and so do not face this difficulty.

5.3 Simulation study

In this section we simulate from Model (3). In addition to the four methods already compared in the previous sections, we can also compare against the Bayes estimator, i.e., group-ridge regression with the oracle choice of regularization parameters (4). We set $p = 800$ and partition the features into $K = 32$ groups (each of size $p_g = 25$). The $g$-th group of features is generated as in (4) with $\alpha_g = (g-1)/31$, i.e., $\alpha_1 = 0$, $\alpha_{32} = 10$ and the other $\alpha_g$s are linearly spaced between 0 and 10. The features are simulated as $x_i \sim \mathcal{N}(0, \Sigma)$ with $\Sigma$ chosen first as the covariance of an autoregressive process of order 1 (AR) with autocorrelation equal to 0.8\textsuperscript{13} and second as the identity matrix. We set $\sigma = 5$ and vary $n \in \{p/2, p, 2p\}$. We also generate 10000 test samples to evaluate the mean

\textsuperscript{13}The correlation persists across blocks, i.e., the covariance is not block-diagonal.
Figure 7: Simulation study: We compare the mean squared error (minus the response noise variance $\sigma^2$) of four methods and the Bayes estimator for two different choices of feature covariance and three different choices of aspect ratio $\gamma \in \{2, 1, 0.5\}$. The $x$-axis shows the number of feature groups $K$ provided to the methods; the side-information is coarser for smaller $K$.

Squared error (MSE). For each setting, we simulate 300 times and report the median MSE across the 300 runs.

In each simulation run, we also coarsen the grouping information as follows: We merge consecutive groups to reduce the total number of groups to $K \in \{2^k \mid k \geq 1\}$. The coarsened grouping information is then passed on to the regression methods used. This coarsening impacts $\sigma$-Ridge, Multi Ridge and the Group Lasso, but not Single Ridge, nor the Bayes estimator.

The results are shown in Figure 7. We make the following observations: Throughout all settings, $\sigma$-Ridge performs best and often gets close to matching the Bayes risk. In some cases, Multi Ridge and Group Lasso have risk close to the one of Single Ridge regression. The results are qualitatively similar across both covariance structures. $\sigma$-Ridge, Multi Ridge and the Group Lasso perform worse when the groups are coarsened to $K = 2$; in this case the side-information made available to them is weak and does not fully capture the heterogeneity of the data-generating mechanism; thus even as $n \to \infty$, these methods would not match the Bayes risk. As $K$ grows, the gap to the Bayes risk becomes smaller. As $K$ becomes even larger (e.g., $K = 32$), however, $\sigma$-Ridge regression (and Multi Ridge) starts to perform worse and this effect is most pronounced when the sample size is small ($n = p/2$). The reason is that the map $\sigma \mapsto \hat{\lambda}_\sigma (11)$ becomes more unstable due to larger estimation error. In the regime depicted in the left-most panels of Figure 7 ($K = 32$, $p_0 = 25$, $\gamma = 2$ and $n = 400$), the asymptotics of Theorem 2 have not kicked in yet, so there is a larger gap to the Bayes risk. Nevertheless, even in this regime, $\sigma$-Ridge outperforms Single Ridge.
6 Discussion

In this paper we have presented an end-to-end approach for implementing group-regularized ridge regression in high dimensions, that is both practical and is supported theoretically. Side-information in regression settings has become ubiquitous in modern applications with large-scale datasets, and its importance is only going to grow in the future. Fortunately, practitioners, already have access to a wealth of practical methods with strong empirical performance [Van De Wiel et al., 2016, Velten and Huber, 2019, Tay et al., 2020]. We hope that our work, will spur further methodological and theoretical developments beyond model (2), for example to classification settings, to other penalties and to more general forms of side-information. Recent theoretical advances in understanding high-dimensional regression and classification [Montanari et al., 2019, Celentano and Montanari, 2019, Liang and Sur, 2020, Taheri et al., 2020a,b] could be instrumental in such an effort. Another avenue of research would be the development of “wrapper” methods that enable the utilization of side-information by black-box supervised learning methods. For example, Ren and Candès [2020] develop methods for feature selection and ranking based on any feature importance statistic and any machine learning model can be enhanced by accounting for side-information.

From a broader methodological perspective, our conceptual approach is the following: we use a model-based/empirical Bayes approach to capture key aspects of the data generating mechanism in a flexible and efficient way (the system (11)); but then we calibrate the result by tuning a 1-dimensional parameter based on a frequentist criterion; in this case the leave-one-out cross-validation error (17). This paradigm –flexible modeling plus calibration of a 1-dimensional parameter based on frequentist criteria– has proven to be fruitful for statistical applications going beyond the group-regularized ridge regression problem considered here. Further applications of this paradigm include feature selection in regression settings via knockoffs [Candès et al., 2018, Ren and Candès, 2020], multiple testing with side-information [Ignatiadis et al., 2016, Lei and Fithian, 2018, Ignatiadis and Huber, 2018], empirical Bayes shrinkage with side-information [Tan, 2016, Ignatiadis and Wager, 2019] and conformal prediction [Vovk et al., 2005, Gupta et al., 2019].

Software

A software package implementing the method is available on Github under the link https://github.com/nignatiadis/SigmaRidgeRegression.jl. The package has been implemented in the Julia programming language [Bezanson et al., 2017] and uses the MLJ [Blaom et al., 2020] interface for supervised learning. The Github repository also provides code to reproduce all numerical results and plots in this manuscript.

Acknowledgements

We thank Michael Celentano, Vaggos Chatziafratis, Iain Johnstone, Kenneth Tay, Stefan Wager and Lexing Ying for enlightening discussions and critical comments on the manuscript. We thank Emmanuel Candès for pointing us to literature on estimation of heritability.

References

Yacine Ait-Sahalia and Dacheng Xiu. Using principal component analysis to estimate a high dimensional factor model with high-frequency data. *Journal of Econometrics*, 201(2):384–399, 2017.
Zhi-Dong Bai and Jack W Silverstein. No eigenvalues outside the support of the limiting spectral distribution of large-dimensional sample covariance matrices. *The Annals of Probability*, 26(1):316–345, 1998.

Linn Cecilie Bergersen, Ingrid K Glad, and Heidi Lyng. Weighted lasso with data integration. *Statistical applications in genetics and molecular biology*, 10(1), 2011.

Thierry Bertin-Mahieux, Daniel P.W. Ellis, Brian Whitman, and Paul Lamere. The Million Song Dataset. In *Proceedings of the 12th International Conference on Music Information Retrieval (ISMIR 2011)*, 2011.

Jeff Bezanson, Alan Edelman, Stefan Karpinski, and Viral B Shah. Julia: A fresh approach to numerical computing. *SIAM review*, 59(1):65–98, 2017.

Anthony D Blaom, Franz Kiraly, Thibaut Lienart, Yiannis Simillides, Diego Arenas, and Sebastian J Vollmer. MLJ: A Julia package for composable machine learning. *arXiv preprint arXiv:2007.12285*, 2020.

Anne-Laure Boulesteix, Riccardo De Bin, Xiaoyu Jiang, and Mathias Fuchs. IPF-LASSO: Integrative-penalized regression with penalty factors for prediction based on multi-omics data. *Computational and mathematical methods in medicine*, 2017, 2017.

Evan A Boyle, Yang I Li, and Jonathan K Pritchard. An expanded view of complex traits: from polygenic to omnigenic. *Cell*, 169(7):1177–1186, 2017.

Peter Bühlmann and Sara Van De Geer. *Statistics for high-dimensional data: methods, theory and applications*. Springer Science & Business Media, 2011.

Emmanuel Candès, Yingying Fan, Lucas Janson, and Jinchi Lv. Panning for gold: ‘model-x’ knockoffs for high dimensional controlled variable selection. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 80(3):551–577, 2018.

Michael Celentano and Andrea Montanari. Fundamental barriers to high-dimensional regression with convex penalties. *arXiv preprint arXiv:1903.10603*, 2019.

Lee H Dicker. Variance estimation in high-dimensional linear models. *Biometrika*, 101(2):269–284, 2014.

Lee H Dicker. Ridge regression and asymptotic minimax estimation over spheres of growing dimension. *Bernoulli*, 22(1):1–37, 2016.

Lee H Dicker and Murat A Erdogdu. Maximum likelihood for variance estimation in high-dimensional linear models. In *Artificial Intelligence and Statistics*, pages 159–167, 2016.

Sascha Dietrich, Małgorzata Oleś, Junyan Lu, Leopold Sellner, Simon Anders, Britta Velten, Bian Wu, Jennifer Hülein, Michelle da Silva Liberio, Tatjana Walther, et al. Drug-perturbation-based stratification of blood cancer. *The Journal of Clinical Investigation*, 128(1):427–445, 2018.

Edgar Dobriban and Yue Sheng. WONDER: Weighted one-shot distributed ridge regression in high dimensions. *Journal of Machine Learning Research*, 21(66):1–52, 2020.

Edgar Dobriban and Stefan Wager. High-dimensional asymptotics of prediction: Ridge regression and classification. *The Annals of Statistics*, 46(1):247–279, 2018.

Dheeru Dua and Casey Graff. UCI machine learning repository, 2020. URL http://archive.ics.uci.edu/ml.
László Erdos and Horng-Tzer Yau. A dynamical approach to random matrix theory. *Courant Lecture Notes in Mathematics*, 28, 2017.

Zhou Fan, Yi Sun, and Zhichao Wang. Principal components in linear mixed models with general bulk. *arXiv preprint arXiv:1903.09592*, 2019.

Chuan-sheng Foo, Chuong B Do, and Andrew Y Ng. Efficient multiple hyperparameter learning for log-linear models. In *Advances in Neural Information Processing Systems*, pages 377–384, 2008.

Jerome Friedman, Trevor Hastie, and Rob Tibshirani. Regularization paths for generalized linear models via coordinate descent. *Journal of statistical software*, 33(1):1, 2010.

Chirag Gupta, Arun K Kuchibhotla, and Aaditya K Ramdas. Nested conformal prediction and quantile out-of-bag ensemble methods. *arXiv*, pages arXiv–1910, 2019.

Trevor Hastie, Andrea Montanari, Saharon Rosset, and Ryan J Tibshirani. Surprises in high-dimensional ridgeless least squares interpolation. *arXiv preprint arXiv:1903.08560*, 2019.

Arthur E Hoerl and Robert W Kennard. Ridge regression: Biased estimation for nonorthogonal problems. *Technometrics*, 12(1):55–67, 1970.

Daniel Hsu, Sham M Kakade, and Tong Zhang. Random design analysis of ridge regression. In *Conference on learning theory*, pages 9–1, 2012.

Nikolaos Ignatiadis and Wolfgang Huber. Covariate powered cross-weighted multiple testing. *arXiv:1701.05179*, 2018.

Nikolaos Ignatiadis and Stefan Wager. Covariate-powered empirical Bayes estimation. In *Advances in Neural Information Processing Systems*, pages 9617–9629, 2019.

Nikolaos Ignatiadis, Bernd Klaus, Judith B Zaugg, and Wolfgang Huber. Data-driven hypothesis weighting increases detection power in genome-scale multiple testing. *Nature methods*, 13(7):577, 2016.

Lucas Janson, Rina Foygel Barber, and Emmanuel Candès. Eigenprism: inference for high dimensional signal-to-noise ratios. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 79(4):1037–1065, 2017.

Jiming Jiang, Cong Li, Debashis Paul, Can Yang, and Hongyu Zhao. On high-dimensional mis-specified mixed model analysis in genome-wide association study. *The Annals of Statistics*, 44 (5):2127–2160, 2016.

Olivier Ledoit and Sandrine Péché. Eigenvectors of some large sample covariance matrix ensembles. *Probability Theory and Related Fields*, 151(1):233–264, 2011.

Lihua Lei and William Fithian. AdaPT: an interactive procedure for multiple testing with side information. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 80(4):649–679, 2018.

Ker-Chau Li. Asymptotic optimality for Cp, CL, cross-validation and generalized cross-validation: discrete index set. *The Annals of Statistics*, pages 958–975, 1987.

Tengyuan Liang and Pragya Sur. A precise high-dimensional asymptotic theory for boosting and min-L1-norm interpolated classifiers. *arXiv preprint arXiv:2002.01586*, 2020.
Sifan Liu and Edgar Dobriban. Ridge regression: Structure, cross-validation, and sketching. In *International Conference on Learning Representations*, 2019.

V. A. Marčenko and L. A. Pastur. The spectrum of random matrices. *Teor. Funkciĭ Funkcional. Anal. i Priložen. Vyp.*, 4:122–145, 1967.

Rosa J Meijer and Jelle J Goeman. Efficient approximate k-fold and leave-one-out cross-validation for ridge regression. *Biometrical Journal*, 55(2):141–155, 2013.

James A. Mingo and Roland Speicher. *Free probability and random matrices*, volume 35 of *Fields Institute Monographs*. Springer, New York; Fields Institute for Research in Mathematical Sciences, Toronto, ON, 2017.

Andrea Montanari, Feng Ruan, Youngtak Sohn, and Jun Yan. The generalization error of max-margin linear classifiers: High-dimensional asymptotics in the overparametrized regime. *arXiv preprint arXiv:1911.01544*, 2019.

Magnus M Münch, Carel FW Peeters, Aad W Van Der Vaart, and Mark A Van De Wiel. Adaptive group-regularized logistic elastic net regression. *Biostatistics*, 2018.

Alexandru Nica and Roland Speicher. *Lectures on the combinatorics of free probability*, volume 335 of *London Mathematical Society Lecture Note Series*. Cambridge University Press, Cambridge, 2006.

Konstantinos Perrakis, Sach Mukherjee, and Alzheimer’s Disease Neuroimaging Initiative. Scalable Bayesian regression in high dimensions with multiple data sources. *Journal of Computational and Graphical Statistics*, pages 1–22, 2019.

Sandipan Pramanik and Xianyang Zhang. Structure adaptive Lasso. *arXiv preprint arXiv:2006.02041*, 2020.

Zhimei Ren and Emmanuel Candès. Knockoffs with side information. *arXiv preprint arXiv:2001.07835*, 2020.

Jack W. Silverstein. Strong convergence of the empirical distribution of eigenvalues of large-dimensional random matrices. *J. Multivariate Anal.*, 55(2):331–339, 1995.

Jack W. Silverstein and Sang-II Choi. Analysis of the limiting spectral distribution of large-dimensional random matrices. *J. Multivariate Anal.*, 54(2):295–309, 1995.

Hossein Taheri, Ramtin Pedarsani, and Christos Thrampoulidis. Fundamental limits of ridge-regularized empirical risk minimization in high dimensions. *arXiv preprint arXiv:2006.08917*, 2020a.

Hossein Taheri, Ramtin Pedarsani, and Christos Thrampoulidis. Sharp asymptotics and optimal performance for inference in binary models. *arXiv preprint arXiv:2002.07284*, 2020b.

Feng Tai and Wei Pan. Incorporating prior knowledge of predictors into penalized classifiers with multiple penalty terms. *Bioinformatics*, 23(14):1775–1782, 2007.

Zhiqiang Tan. Steinized empirical Bayes estimation for heteroscedastic data. *Statistica Sinica*, pages 1219–1248, 2016.

Shaozhe Tao, Yifan Sun, and Daniel Boley. Inverse covariance estimation with structured groups. In *IJCAI*, pages 2836–2842, 2017.
Terence Tao. \textit{Topics in random matrix theory}, volume 132 of \textit{Graduate Studies in Mathematics}. American Mathematical Society, Providence, RI, 2012.

J Kenneth Tay, Nima Aghaeepour, Trevor Hastie, and Robert Tibshirani. Feature-weighted elastic net: using\textsuperscript{2} features of features\textsuperscript{2} for better prediction. \textit{arXiv preprint arXiv:2006.01395}, 2020.

Robert Tibshirani. Regression shrinkage and selection via the lasso. \textit{Journal of the Royal Statistical Society: Series B (Methodological)}, 58(1):267–288, 1996.

Andrei Nikolaevich Tikhonov. On the solution of ill-posed problems and the method of regularization. In \textit{Doklady Akademii Nauk}, volume 151, pages 501–504. Russian Academy of Sciences, 1963.

Antonia M Tulino and Sergio Verdú. Random matrix theory and wireless communications. \textit{Foundations and Trends\textregistered in Communications and Information Theory}, 1(1):1–182, 2004.

Mark A Van De Wiel, Tonje G Lien, Wina Verlaat, Wessel N van Wieringen, and Saskia M Wilting. Better prediction by use of co-data: adaptive group-regularized ridge regression. \textit{Statistics in Medicine}, 35(3):368–381, 2016.

Mark A. van de Wiel, Mirrelijn M. van Nee, and Armin Rauschenberger. Fast cross-validation for multi-penalty ridge regression. \textit{arXiv}, 2020.

Wessel N van Wieringen. Lecture notes on ridge regression. \textit{arXiv preprint arXiv:1509.09169v6}, 2020.

Jurre R Veerman, Gwenaël GR Leday, and Mark A van de Wiel. Estimation of variance components, heritability and the ridge penalty in high-dimensional generalized linear models. \textit{Communications in Statistics-Simulation and Computation}, pages 1–19, 2019.

Britta Velten and Wolfgang Huber. Adaptive penalization in high-dimensional regression and classification with external covariates using variational Bayes. \textit{Biostatistics}, 2019.

André Verissimo, Arlindo Limede Oliveira, Marie-France Sagot, and Susana Vinga. DegreeCox–a network-based regularization method for survival analysis. \textit{BMC bioinformatics}, 17(16):449, 2016.

Vladimir Vovk, Alex Gammerman, and Glenn Shafer. \textit{Algorithmic learning in a random world}. Springer Science & Business Media, 2005.

Simon N Wood. Modelling and smoothing parameter estimation with multiple quadratic penalties. \textit{Journal of the Royal Statistical Society: Series B (Statistical Methodology)}, 62(2):413–428, 2000.

Simon N Wood. Stable and efficient multiple smoothing parameter estimation for generalized additive models. \textit{Journal of the American Statistical Association}, 99(467):673–686, 2004.

Simon N Wood. \textit{Generalized additive models: an introduction with R}. CRC press, 2017.

Denny Wu and Ji Xu. On the optimal weighted $\ell_2$ regularization in overparameterized linear regression. \textit{arXiv preprint arXiv:2006.05800}, 2020.

Ji Xu and Daniel J Hsu. On the number of variables to use in principal component regression. In \textit{Advances in Neural Information Processing Systems}, pages 5095–5104, 2019.

Ji Xu, Arian Maleki, and Kamri Rahnama Rad. Consistent risk estimation in high-dimensional linear regression. \textit{arXiv preprint arXiv:1902.01753}, 2019.
Jianfeng Yao, Shurong Zheng, and Zhidong Bai. *Large sample covariance matrices and high-dimensional data analysis*, volume 39 of *Cambridge Series in Statistical and Probabilistic Mathematics*. Cambridge University Press, New York, 2015. ISBN 978-1-107-06517-8.

Ming Yuan and Yi Lin. Model selection and estimation in regression with grouped variables. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 68(1):49–67, 2006.

Chubing Zeng, Duncan Campbell Thomas, and Juan Pablo Lewinger. Incorporating prior knowledge into regularized regression. *Bioinformatics*, 2020.

Fan Zhou and Iain M Johnstone. Eigenvalue distributions of variance components estimators in high-dimensional random effects models. *Annals of Statistics*, 47(5):2855, 2019.
A Proofs for Section 2

Proof of Proposition 1.

1. Note that we are minimizing $\|Ad(\sigma) - b(\sigma)\|_2$, where $b_g(\sigma) = \hat{u}_g / \sigma^2 - v_g$. In particular, when $\sigma^2 \geq \hat{u}_g / v_g$ for all $g$, then $b_g(\sigma) \leq 0$ for all $g$. But since all entries of $A$ are $\geq 0$ and we optimize over $d(\sigma) \in [0, \infty)^K$, the lowest objective value must be attained when $d(\sigma) = 0$ and so all $\hat{\lambda}_g(\sigma) = \infty$.

2. Let us introduce dual variables $\zeta(\sigma) \geq 0$, then the Lagrangian takes the form:

$$L(d(\sigma); \zeta(\sigma)) = \|Ad(\sigma) - b(\sigma)\|_2^2 - d(\sigma)^T \zeta(\sigma)$$

Minimizing with respect to $d(\sigma)$ we find that:

$$A^T Ad(\sigma) = A^T b(\sigma) + \zeta(\sigma) / 2 =: \eta(\sigma)$$

Note that $b_g(\sigma) \to \infty$ as $\sigma \to 0$, and so, since all entries of $A$ are $\geq 0$ and $A$ is invertible, it also follows that $\eta_g(\sigma) \to \infty$ as $\sigma \to 0$. Now let $a^* > 0$ be the largest entry of $A^T A$, then it follows that (for all $k \in \{1, \ldots, K\}$):

$$\max_g \left\{ \hat{d}_g(\sigma) \right\} \cdot a^* \cdot K \geq \eta_k(\sigma)$$

Thus $\max_g \left\{ \hat{d}_g(\sigma) \right\} \to \infty$ as $\sigma \to 0$, i.e., $\min_g \left\{ \hat{\lambda}_g(\sigma) \right\} \to 0$.

3. Let $S_j \subset \{1, \ldots, K\}$ be the subset of coordinates $g$ so that $\hat{d}_g(\sigma) > 0$ (and so $\hat{\lambda}_g(\sigma) < \infty$). Then from the Karush-Kuhn-Tucker (KKT) conditions (30) holds and furthermore (by complementary slackness) $\zeta_g(\sigma) = 0$ for all $g \in S_j$. Hence, subsetting (30) to $S_j$ and letting $M_j = A^T_{i, S_j} A_{i, S_j}$ we get

$$M_j d_S(\sigma) = A^T_{i, S_j} b(\sigma)$$

Thus for a local perturbation of $\sigma$, there will remain a solution $d_{S_j}(\tilde{\sigma})$ to the above system with all coordinates $> 0$ and hence will satisfy the KKT conditions for the optimization problem at $\tilde{\sigma}$.

Now let $\sigma_2, \sigma_1 \in I_j$, then:

$$M_j d_S(\sigma_1) = A^T_{i, S_j} \left( u / \sigma_1^2 - v \right)$$

$$= \frac{\sigma_2}{\sigma_1^2} A^T_{i, S_j} \left( u / \sigma_2^2 - v \right) + \left( \frac{\sigma_2}{\sigma_1^2} - 1 \right) A^T_{i, S_j} v$$

$$= \frac{\sigma_2}{\sigma_1^2} M_j d_S(\sigma_2) + \left( \frac{\sigma_2}{\sigma_1^2} - 1 \right) A^T_{i, S_j} v$$

By multiplying with $M_j^{-1}$ we conclude.

B Proofs for Section 3, Lemma 1

We will need the following lemma which is adapted from Lemma 7.8, Lemma 7.9 and Lemma 7.10 from Erdos and Yau [2017]. This will be an essential ingredient in controlling the concentration of quadratic forms that we will encounter.

Lemma 4. Let $q \geq 2$ and $X_1, \ldots, X_N, Y_1, \ldots, Y_N$ be independent random variables with mean 0, variance 1 and $2q$-th moment bounded by $c_0$. Then, for any deterministic $(b_i)_{1 \leq i \leq N}, (a_{ij})_{1 \leq i, j \leq N}$ we have for some positive constant $C_q = C_q(c_0)$.
\[
\left\| \sum_i b_i (X_i^2 - 1) \right\|_q \leq C_q \left( \sum_i |b_i|^2 \right)^{\frac{1}{q}},
\]

\[
\left\| \sum_{i,j} a_{ij} X_i Y_j \right\|_q \leq C_q \left( \sum_{i,j} a_{ij}^2 \right)^{\frac{1}{2}},
\]

\[
\left\| \sum_{i \neq j} a_{ij} X_i X_j \right\|_q \leq C_q \left( \sum_{i \neq j} a_{ij}^2 \right)^{\frac{1}{2}},
\]

where \( \| \cdot \|_q \) is the \( L_q \) norm, i.e., \( \| U \|_q = \mathbb{E}[|U|^q]^{1/q} \) for a random variable \( U \).

**Proof of Lemma 1.** Assume that pointwise convergence holds (which we will prove later). We show that it can be extended to uniform convergence on a compact set \( C \subset (0, \infty)^K \) which we fix. First, note that

\[
\hat{w} = \left( \frac{X^\top X}{n} + \Lambda \right)^{-1} \frac{X^\top Y}{n} \]

\[
= w - \left( \frac{X^\top X}{n} + \Lambda \right)^{-1} \Lambda w + \left( \frac{X^\top X}{n} + \Lambda \right)^{-1} \frac{X^\top \varepsilon}{n}\]

\[
= A \frac{\varepsilon}{\sqrt{n}} + w - B w, \quad \text{with} \quad A = \left( \frac{X^\top X}{n} + \Lambda \right)^{-1} \frac{X^\top \varepsilon}{\sqrt{n}}, \quad B = \left( \frac{X^\top X}{n} + \Lambda \right)^{-1} \Lambda.
\]

By the strong law of large numbers, we have that \( \| w \|^2 \overset{a.s.}{\longrightarrow} \sum_{i=1}^K \alpha_i^2 < \infty \) and \( \| \varepsilon \|^2 \overset{a.s.}{\longrightarrow} \sigma^2 \). In addition, for \( \Lambda \in C \) it holds that

\[
\| B \| \leq 1
\]

and also that

\[
\| A \| \leq \left\| \frac{X}{\sqrt{n}} \right\| \times \left\| \left( \frac{X^\top X}{n} + \Lambda \right)^{-1} \right\| \leq \| \Sigma \|^{\frac{1}{2}} \times \left\| \frac{Z}{\sqrt{n}} \right\| \| \Lambda^{-1} \|.
\]

Using \( \lim_{n \to \infty} \| Z/\sqrt{n} \| = 1 + \sqrt{7} \) [Bai and Silverstein, 1998] we get that almost surely

\[
\lim \sup_{\lambda \in C} \max_{\Lambda \in \mathcal{C}} \| A \| < \infty
\]

(36)

Combining (35) and (36) we conclude that almost surely

\[
\lim \sup_{\lambda \in C} \max_{\Lambda \in \mathcal{C}} \| \hat{w}(\lambda) - w \| < \infty.
\]

By a very similar argument we get that almost surely

\[
\lim \sup_{\lambda \in C} \max_{\Lambda \in \mathcal{C}} \| \nabla_\Lambda \hat{w}(\lambda) \| < \infty.
\]

Since \( R_n = \sigma^2 + (\hat{w} - w) \Sigma (\hat{w} - w) \), we have by the previous observations that

\[
\lim \sup_{\lambda \in C} \max_{\Lambda \in \mathcal{C}} \| \nabla_\Lambda R_n(\lambda) \| < \infty.
\]

Hence, the sequence of functions \( \{ R_n \}_{n \geq 1} \) is almost surely uniformly bounded and equicontinuous on \( C \). Similarly for the sequence \( \{ L_n \}_{n \geq 1} \), hence for the difference \( F_n = R_n - L_n \). Since \( F \overset{a.s.}{\longrightarrow} 0 \)

29
on a countable dense subset, the only uniform subsequential limit of \( F_n \) can be the function 0. Due to the fact that almost surely any subsequence of \( \{ F_n \}_{n \geq 1} \) has a uniformly convergent subsequence by the Arzela-Ascoli theorem, we conclude that it must almost surely converge uniformly to 0.

It remains to show pointwise convergence. With the same notation as above

\[
(\hat{w} - w)^\top \Sigma (\hat{w} - w) = \frac{\varepsilon^\top A^\top \Sigma A \varepsilon}{n} + w^\top B^\top \Sigma B w - \frac{2 \varepsilon^\top A^\top \Sigma B w}{\sqrt{n}}.
\]

Using Lemma 4 for \( q = (4 + \eta)/2 \) for the three quadratic forms in the expression above we see (details below) that:

\[
\frac{\varepsilon^\top A^\top \Sigma A \varepsilon}{n} \overset{a.s.}{\to} 0,
\]

\[
\frac{\varepsilon^\top A^\top \Sigma B w}{\sqrt{n}} \overset{a.s.}{\to} 0,
\]

\[
w^\top B^\top B w - \frac{1}{p} \text{Tr} \left( \left( \frac{X^\top X}{n} + \Lambda \right)^{-1} \Sigma \left( \frac{X^\top X}{n} + \Lambda \right)^{-1} \Lambda \bar{D} \Lambda \right) \overset{a.s.}{\to} 0.
\]

From the last three convergence results pointwise convergence of \( R_n - L_n \) follows. The proof is completed, once we justify the three almost sure limits above. We provide the details for the second limit; the argument for the other two cases is almost identical. Using Lemma 4 after taking into account the variances of \( \varepsilon, w \) we have

\[
\frac{\| \varepsilon^\top A^\top \Sigma B w \|_q}{\sqrt{n}} = O \left( (pn)^{-\frac{q}{2}} \| A^\top \Sigma B \|_F \right) = O \left( (pn)^{-\frac{q}{2}} \| \Sigma \| \| B \| \| A \| \sqrt{p} \right) = O(n^{-\frac{q}{2}}).
\]

It follows by Markov’s inequality that, for any \( \epsilon > 0 \),

\[
P \left( \left| \frac{\varepsilon^\top A^\top \Sigma B w}{\sqrt{n}} \right| > \epsilon \right) \leq \epsilon^{-q} \frac{\| \varepsilon^\top A^\top \Sigma B w \|_q^q}{n^2} = O \left( n^{-\frac{q}{2}} \right).
\]

Since \( q/2 = 1 + \eta/4 > 1 \), by Borel-Cantelli we know that with probability 1 eventually

\[
\left| \frac{\varepsilon^\top A^\top \Sigma B w}{\sqrt{n}} \right| < \epsilon.
\]

This proves the desired convergence, since \( \epsilon \) was arbitrary.

\[\square\]

C Proofs for Section 3: Risk formulae

C.1 Preliminaries from Random Matrix theory and Free Probability

We provide a short review of some tools from free-probability that we are going to use in the proofs in the next subsection. For a comprehensive introduction to free-probability and proofs for the results that are mentioned here, the reader can refer to Mingo and Speicher [2017] and Nica and Speicher [2006]. In the last decade the emergence of random matrix theory in statistics has made free-probability methods very fruitful; see for example Fan, Sun, and Wang [2019] and Zhou and Johnstone [2019].

For a probability measure \( \mu \) on the real line, we define the Stieltjes transform \( m_\mu(z) = \int \frac{\mu(dx)}{x-z} \) for \( z \in \mathbb{C} \) away from the support of \( \mu \). This is a holomorphic function and \( m_\mu(z) \in \mathbb{C}^+ \) if and only if \( z \in \mathbb{C}^+ \).
Before we start with the free-probability tools that we need, we refer to the famous generalized Marcenko-Pastur distribution. For a real symmetric matrix with eigenvalues $\sigma_1, \ldots, \sigma_p$ (including multiplicity), the empirical spectral distribution is the probability measure on the real line defined as $\frac{1}{p} \sum_{j=1}^{p} \delta_{\sigma_j}$. For the empirical covariance matrix of i.i.d. random variables $x_1, \ldots, x_n$ with $x_i = \Sigma^{1/2} z_i$, where $z_i$ has mean 0-variance 1 i.i.d. entries, $p, n \to \infty$ and $\frac{p}{n} \to \gamma > 0$, it is well-known that the empirical spectral distribution has a weak limit if $\Sigma$ is either nonrandom or independent of $z_i$’s and has itself a limiting spectral distribution $H$. In particular, we have the following famous result:

**Theorem** (Marcenko and Pastur [1967] and Silverstein [1995]). The empirical spectral distribution of the empirical covariance matrix converges almost surely to a deterministic measure with Stieltjes transform $m_{\gamma,H}$ that satisfies

$$m_{\gamma,H}(z) = \int \frac{dH(t)}{t(1 - \gamma - \gamma zm_{\gamma,H}) - t - z}.$$

For the null case $H = \delta_1$ we get the standard Marcenko-Pastur distribution with parameter $\gamma$. This is a probability measure that has density

$$p_{\gamma}(x) = \frac{\sqrt{(b_{\gamma} - x)(x - a_{\gamma})}}{2\pi\gamma x}, \quad a_{\gamma} < x < b_{\gamma}.$$

The support is given by $a_{\gamma} = (1 - \sqrt{\gamma})^2$, $b_{\gamma} = (1 + \sqrt{\gamma})^2$. In the case of $\gamma \geq 1$ we get an extra mass of size $1 - \frac{1}{\gamma}$ at 0.

If we know the Stieltjes transform of the limiting spectral distribution, the density (assuming it exists) can be recovered by the Stieltjes inversion formula:

$$p(x) = \frac{1}{\pi} \lim_{u \downarrow 0} \text{Im}(m_{\gamma,H}(x + iu)).$$

Asymptotic freeness plays a major role for our proofs and we define it here following Mingo and Speicher [2017] and Tao [2012]. We will use $\tau(W) = \frac{1}{N} \text{Tr}(W)$ to denote the normalized trace of an $N \times N$ matrix $W$, $\tau(W) = \mathbb{E}[\tau(W)]$.

**Definition 1** (Definition 2.5.18 in Tao [2012]). Consider two sequences of $N \times N$ random matrices $(A_N)_{N \geq 1}, (B_N)_{N \geq 1}$. We call them asymptotically freely independent when for each $m \in \mathbb{N}$ and any polynomials $P_1, \ldots, P_m$ we have

$$\tau(\Pi_{i=1}^{m}(P_i(C_i) - \tau(P_i(C_i)))) \xrightarrow{N \to \infty} 0,$$

where $C_1, \ldots, C_m$ is any alternating choice of $A_N, B_N$. If the same convergence holds with $\tau$ instead of $\tau$, i.e., if,

$$\tau(\Pi_{i=1}^{m}(P_i(C_i) - \tau(P_i(C_i)))) \xrightarrow{N \to \infty} 0, \text{ almost surely},$$

then we say that the sequences of matrices are almost surely asymptotically free.

A well-known result from Mingo and Speicher [2017] is the following.

**Theorem** (Page 111 in Mingo and Speicher [2017]). Let $A_N$ and $B_N$ be two sequences of independent $N \times N$ matrices that converge almost surely in moments to some probability measures. Let $U_N$ be a matrix drawn independently from $A_N, B_N$ with respect to the Haar measure. Then, $A_N, U_N^{-1} B_N U_N$ are almost surely asymptotically free.
If $\mu$ has compact support, it is well-known that there exists a function $R_\mu$ which is holomorphic in some open set containing 0 for which $m_\mu(R_\mu(z) + \frac{1}{z}) = z$. We will use the notation $B_\mu(-z) = R_\mu(z) + \frac{1}{z}$.

We have the following result from Mingo and Speicher [2017].

**Theorem** (Page 51 in Mingo and Speicher [2017]). Let $A, B$ be independent symmetric $N \times N$ random matrices and $U$ an independent random matrix which is uniformly distributed with respect to the Haar measure on $\mathbb{R}^{N \times N}$. If the empirical spectral distributions of $A, B$ converge to deterministic probability measures $\mu, \nu$ respectively, then the empirical spectral distribution of the matrix $A + U^*BU$ converges almost surely to a measure with R-transform $R(z) = R_\mu(z) + R_\nu(z)$.

This is known as the free additive convolution of $\mu, \nu$.

### C.2 Proofs of the risk formulas

Throughout this section, we assume without loss of generality that the features are indexed so that $\mathcal{G}_1 = \{1, \ldots, p_1\}$, $\mathcal{G}_2 = \{p_1 + 1, \ldots, p_1 + p_2\}$ and so forth. Second, given a $\lambda = (\lambda_1, \ldots, \lambda_K) \in [0, \infty]^K$ we will write $\Lambda$ for the diagonal $p \times p$ matrix with diagonal $(\lambda_1, \ldots, \lambda_1, \lambda_2, \ldots, \lambda_{K-1}, \lambda_K, \ldots, \lambda_K)$.

We start with some preliminary observations. First, letting $M = \left( \frac{Z^*Z}{n} + \Sigma^{-\frac{1}{2}}\Lambda\Sigma^{-\frac{1}{2}} \right)^{-1}$, it holds that

$$\partial_j M = -M \begin{pmatrix} 0_{p_1} & \cdots & 0_{p_K} \\ \Sigma_j^{-1} & \ldots & \Sigma_j^{-1} \end{pmatrix} M.$$  

(37)

Using Lemma 1, it suffices to study the asymptotics of $L(\lambda)$ and so it suffices to study:

$$1 + \frac{1}{n} \text{Tr} \left( \frac{X^*X}{n} \left( \frac{X^*X}{n} + \Lambda \right)^{-1} \Sigma \left( \frac{X^*X}{n} + \Lambda \right)^{-1} \right)$$

$$+ \frac{1}{p} \text{Tr} \left( \left( \frac{X^*X}{n} + \Lambda \right)^{-1} \Sigma \left( \frac{X^*X}{n} + \Lambda \right)^{-1} \Lambda D\Lambda \right).$$

We study the two non-constant terms separately. The first term can be rewritten as

$$\frac{1}{n} \text{Tr} \left( \left( \frac{X^*X}{n} + \Lambda \right)^{-1} \Sigma \right) - \frac{1}{n} \text{Tr} \left( \left( \frac{X^*X}{n} + \Lambda \right)^{-1} \Sigma \left( \frac{X^*X}{n} + \Lambda \right)^{-1} \Lambda \right)$$

$$= \frac{1}{n} \text{Tr} \left( \Sigma^{-\frac{1}{2}}M\Sigma^{-\frac{1}{2}} \Sigma \right) - \frac{1}{n} \text{Tr} \left( \Sigma^{-\frac{1}{2}}M\Sigma^{-\frac{1}{2}} \Sigma \Sigma^{-\frac{1}{2}}M\Sigma^{-\frac{1}{2}} \Lambda \right)$$

$$= \frac{1}{n} \text{Tr}(M) - \frac{1}{n} \text{Tr} \left( M^2 \Sigma^{-1} \Lambda \right),$$

where in the last equality we have used the fact that $\Sigma, \Lambda$ commute. Also notice that

$$\text{Tr} \left( M^2 \Sigma^{-1} \Lambda \right) = \text{Tr} \left( M \Sigma^{-1} M \right) = -\sum_{j=1}^k \lambda_j \text{Tr}(\partial_j M).$$

32
Combining everything and also noting that replacing $n$ by $\gamma/p$ only changes an $o(1)$ term, we see that the first term can be rewritten as

$$\gamma \frac{1}{p} \text{Tr} \left( M + \sum_{j=1}^{k} \lambda_j \partial_j M \right) + o(1).$$

The second term can be rewritten as

$$\frac{1}{p} \text{Tr} \left( \Sigma^{-\frac{1}{2}} M \Sigma^{-\frac{1}{2}} \Sigma^{-\frac{1}{2}} \Lambda \Sigma^{-\frac{1}{2}} \Lambda D \Lambda \right) = \frac{1}{p} \text{Tr} \left( M^2 \Sigma^{-1} \Lambda^2 D \right),$$

where also here we used the fact that $D, \Lambda, \Sigma$ commute with each other. This can be rewritten as

$$\frac{1}{p} \text{Tr} \left( M \Sigma^{-\frac{1}{2}} \Lambda \Sigma^{-\frac{1}{2}} \right) = -\frac{1}{p} \text{Tr} \left( \sum_{j=1}^{K} \frac{\gamma}{\gamma_j} \alpha_j^2 \lambda_j \partial_j M \right) + o(1).$$

We conclude that the risk can be approximated by (up to $o(1)$ terms) by

$$1 + \frac{1}{p} \text{Tr} \left( \gamma M + \sum_{j=1}^{K} \frac{\gamma}{\gamma_j} (\gamma_j \lambda_j - \alpha_j^2 \lambda_j) \partial_j M \right).$$

Our remaining goal is to more precisely characterize the limit of the above expression.

**Proposition 2.** We have for $z \in \mathbb{C} - \mathbb{R}$

$$\frac{1}{n} \text{Tr} \left( \frac{Z^\top Z}{n} + \Sigma^{-\frac{1}{2}} \Lambda \Sigma^{-\frac{1}{2}} - z \right)^{-1} \to m(z),$$

where

$$m(z) = \sum_{j=1}^{k} \frac{\gamma_j}{\gamma} \int \left( \frac{\lambda_j}{t} - z + \frac{1}{1 + \gamma m(z)} \right)^{-1} dH_j(t)$$

and $\text{Im}(z) \text{Im}(m(z)) > 0$. In other words, the empirical spectral distribution of

$$\frac{Z^\top Z}{n} + \Sigma^{-\frac{1}{2}} \Lambda \Sigma^{-\frac{1}{2}}$$

converges to a probability measure $\mu$ with Stieltjes transform $m(z) = \int \frac{1}{z-x} \mu(dx)$ described by the equation above.

**Proof.** We know that the empirical spectral distribution of $Z^\top Z/n$ converges almost surely to the Marcenko-Pastur distribution with parameter $\gamma$, which has a Stieltjes transform $m_{\gamma}(z)$ that satisfies

$$m_{\gamma}(z) = \frac{1}{1 - \gamma - z - \gamma m_{\gamma}(z)}.$$  
Solving $m_{\gamma}(B_1(z)) = -z$ gives $B_1(z) = \frac{1}{z} + \frac{1}{1 + \gamma z}$, so the R-transform of the Marcenko-Pastur distribution is $B_1(z) = \frac{1}{1 + \gamma z}$. From our assumptions, it is clear that the empirical spectral distribution of $\Sigma^{-\frac{1}{2}} \Lambda \Sigma^{-\frac{1}{2}}$ also converges to a deterministic measure which we call $\nu$. If $U$ is uniformly distributed with respect to the Haar measure, then $U Z^\top Z U^\top$ has the same distribution as $U Z^\top Z U^\top$. We see that the empirical spectral distribution of

$$\frac{Z^\top Z}{n} + \Sigma^{-\frac{1}{2}} \Lambda \Sigma^{-\frac{1}{2}}$$
converges almost surely to a measure with R-transform

\[ R(z) = R_1(z) + R_\nu(z) = \frac{1}{1 - \gamma z} + R_\nu(z) \implies B(z) = \frac{1}{1 - \gamma z} + B_\nu(z). \]

If \( m \) is the Stieltjes transform of the limit, we get that \( z = 1/(1 + \gamma m(z)) + B_\nu(-m(z)) \) and so by change of variables, we get:

\[ m(z) = m_\nu \left( z - \frac{1}{1 + \gamma m(z)} \right) = \sum_{j=1}^K \frac{\gamma_j}{\gamma} \int \left( \frac{\lambda_j}{t} - z + \frac{1}{1 + \gamma m(z)} \right)^{-1} dH_j(t). \]

\[ \square \]

**Proof of Theorem 1.** As a first consequence of Proposition 2, we observe that by taking \( z \to 0 \), it follows that

\[ \frac{1}{p} \text{Tr}(M) \xrightarrow{a.s.} m(0). \quad (38) \]

Here we used the fact that the spectrum of \( Z^{-\frac{1}{2}}Z + \Sigma^{-\frac{1}{2}} \Lambda \Sigma^{-\frac{1}{2}} \) is bounded away from zero. In the statement of our theorem, \( m(0) \) will play the role of \( f = f(\lambda) = m(0) \). Writing \( M \) also as a function of \( \lambda \), i.e., \( M = M(\lambda) = M(\lambda_1, \ldots, \lambda_K) \), we thus have proven convergence

\[ \frac{1}{p} \text{Tr}(M(\lambda)) \xrightarrow{a.s.} f(\lambda), \quad (39) \]

To conclude, it suffices to show that

\[ \frac{1}{p} \text{Tr}(\partial_1 M(\lambda)) \xrightarrow{a.s.} \partial_1 f(\lambda), \quad (40) \]

and similarly for the other groups. \((39)\), however does not directly imply \((40)\), since a sequence of functions can converge almost surely to a deterministic function, but the sequence of derivatives may not converge. We now work to circumvent this problem. We prove the convergence for the partial derivative with respect to \( \lambda_1 \) and similarly one can prove the convergence of the other partial derivatives.

We claim the following slight generalization of Proposition 2, which we will verify later.

**Claim:** For \( z \in \mathbb{C} \) in a neighborhood of the fixed \( \lambda_1 > 0 \), it holds that almost surely \( h_p(z) = \frac{1}{p} \text{Tr}(M(z, \lambda_2, \ldots, \lambda_K)) \) converges to a function \( h_\infty(z) \). \( h_\infty(z) \) depends on \( \lambda_2, \ldots, \lambda_k \), but for notational simplicity we suppress this dependency.

Now, let \( \Gamma \) be a circle contained in that neighborhood of \( \lambda_1 \). Considering a countable dense subset \( \tilde{\Gamma} \) of \( \Gamma \), then we know that almost surely \( h_p(z) \to h_\infty(z) \) for all \( z \in \tilde{\Gamma} \).

Next, observe that

\[ |h_p'(z)| \leq \left\| M(z, \lambda_2, \ldots, \lambda_K) \left( \Sigma^{-1} \right)_{p-p_1} M(z, \lambda_2, \ldots, \lambda_K) \right\| \leq \| \Sigma^{-1} \| \| M(z, \lambda_2, \ldots, \lambda_K) \|^2 \]

is uniformly bounded for \( z \in \mathbb{C} \) close to \( \lambda_1 \), say by some constant \( \tilde{C} \) independent of \( p \). We conclude that

\[ |h_p(z_2) - h_p(z_1)| \leq \int_0^1 |h'_p(tz_2 + (1 - t)z_1)| \, dt \, |z_2 - z_1| \leq \tilde{C} \, |z_2 - z_1| \]

for \( z_1, z_2 \) in a neighborhood of \( \lambda_1 \). As a result the, the functions \( h_p(z) \) are uniformly bounded and equicontinuous. Thus, \( h_p \) has a subsequence that converges uniformly by the Arzela-Ascoli
the risk is asymptotically equal to $1 + \gamma g$ asymptotically optimal choice of regularization parameters. For this choice of optimal parameters $L$ generally. By equicontinuity of mean of the distribution of $P$ this implies that the Bayes optimal parameters $\delta > 0$.

Since $Z$ depend on the distribution of $w$ let $\lambda$.

Proof of Corollary 2. Let $g(\lambda) = f(\lambda, \lambda, \cdots, \lambda)$. Then,

$$g'(\lambda) = -\int \frac{tdH(t)}{(\lambda + \frac{t}{1+\gamma})^2} + \gamma g'(\lambda) \int \frac{dH(t)}{(1 + \lambda + \gamma g)^2}. $$

We set

$$T_1(\lambda) = \int \frac{tdH(t)}{(\lambda + \frac{t}{1+\gamma})^2}, \quad T_2(\lambda) = -1 + \gamma \int \frac{dH(t)}{(1 + \lambda + \gamma g)^2}. $$

$$h_p(z) = \frac{1}{2\pi i} \oint \frac{h_p(w)}{(w - z)^2} dw.$$
Then, $g'(\lambda) = T_1(\lambda)T_2(\lambda)^{-1}$. For the partial derivatives $\partial_\lambda f(\lambda, \cdots, \lambda)$ we find

$$
\partial_\lambda f(\lambda, \lambda, \cdots, \lambda) = -\frac{\gamma_1}{\gamma} \int \frac{tdH(t)}{(\lambda + \frac{t}{1+\gamma})^2} + \partial_\lambda f(\lambda, \lambda, \cdots, \lambda) \sum_{j=1}^k \gamma_j \int \frac{dH(t)}{1+\lambda \frac{t}{1+\gamma}}^2,
$$

and so

$$
\partial_\lambda f(\lambda, \lambda, \cdots, \lambda) = \frac{\gamma_1}{\gamma} T_1(\lambda)T_2^{-1}(\lambda) = \frac{\gamma_1}{\gamma} g'(\lambda).
$$

This implies that the risk is asymptotically

$$
1 + \gamma g(\lambda) + \sum_{i=1}^K (\gamma \lambda - \alpha_i^2 \lambda^2)g'(\lambda) = 1 + \gamma g(\lambda) + (\gamma \lambda - \alpha^2 \lambda^2)g'(\lambda),
$$

where $\alpha^2 = \alpha_1^2 + \cdots \alpha_K^2$. As a result, the risk in this case is equal to the risk of ridge regression in a model with only 1 group and variance of each individual weight equal to $\alpha^2 p^{-1}$. The value of $\lambda$ that minimizes this is $\lambda^* = \frac{\alpha}{\alpha^*}$ by Corollary 1.

**Proof of Corollary 3.** Let $u = (1 + \gamma f)^{-1}$. Then,

$$
\frac{1}{u} = 1 + \sum_{j=1}^K \gamma_j \frac{1}{\lambda_j + u} \Rightarrow \frac{\partial_{\lambda_1} u}{u^2} = \sum_{j=1}^K \frac{\gamma_j \partial_{\lambda_1} u}{(\lambda_j + u)^2} + \frac{\gamma_1}{(\lambda_1 + u)^2}.
$$

For $\lambda_1 = \cdots = \lambda_K = \lambda$ we get (suppressing the dependency of $u$ on $\lambda$ in the equations below)

$$
\partial_{\lambda_1} u(\lambda, \cdots, \lambda) = \frac{\gamma_1 u^2}{(\lambda + u)^2 - \gamma u^2}
$$

$$
\Rightarrow \partial_{\lambda_1} f(\lambda, \cdots, \lambda) = -\frac{1}{\gamma} \frac{\partial_{\lambda_1} u(\lambda, \cdots, \lambda)}{u^2} = \frac{\gamma_1}{\gamma} \frac{1}{\gamma u^2 - (\lambda + u)^2}.
$$

Upon repeating this argument for all groups $g$, Theorem 1 implies that the asymptotic risk is

$$
\frac{1}{u} - \frac{\gamma \lambda - (\sum_{j=1}^K \alpha_j^2) \lambda^2}{(\lambda + u)^2 - \gamma u^2}.
$$

We next solve

$$
\frac{1}{u} = 1 + \frac{\gamma}{\lambda + u} \Rightarrow u = \frac{1 - \gamma - \lambda + \sqrt{(\lambda + \gamma - 1)^2 + 4 \lambda}}{2}.
$$

Finally, applying Corollaries 1 and 2 we find that the optimal risk (based on a single $\lambda$) is given by

$$
\frac{\gamma + \lambda^* - 1 + \sqrt{\gamma + \lambda^* - 1)^2 + 4 \lambda^*}}{2 \lambda^*}.
$$

**Proof of Corollary 4.** Since most of the work has already been done, we sketch the proof only. The problem if we ignore the second problem becomes equivalent to our original problem, but with only one group and residual variance $1 + \alpha_2^2$. Thus, the Bayes optimal parameter in this scenario becomes $\hat{\lambda} = \gamma_1 (\alpha_2^2 + 1)/\alpha_2^2$ which gives the posterior mean for any $n$. In other words, the problem is the same as in the case $K = 1$, but the error has to be rescaled by $1 + \alpha_2^2$ and the variance of the weights has to be divided by that number exactly to compensate for that. The result then follows by Corollary 3.
We now also prove the two remarks following the statement of the corollary. To see why the first remark ($\gamma < 1$) holds, we take $\alpha \to \infty$, so $\tilde{\lambda}, \lambda^* \to 0$. The LHS in the last inequality of the statement of Corollary 4 converges to $\frac{1}{1-\gamma}$, while the RHS converges to $\frac{\alpha^2 + 1}{1-\gamma}$. Now we solve

$$\frac{\alpha^2 + 1}{1-\gamma} \leq \frac{1}{1-\gamma} \implies \alpha^2 \leq \frac{\gamma^2}{1-\gamma}.$$ 

If $\alpha^2$ exceeds the threshold $\sqrt{\frac{\gamma^2}{(1-\gamma)}}$, then the performance in the case that we know the values of the predictors in the second group is enhanced by including them, even if we use a single regularization parameter.

For the second remark, we consider the case $\gamma^* > 1$ (the case $\gamma^* \leq 1$ being similar). The LHS in (25) grows as $(\gamma - 1)/\lambda^*$, while the RHS as $(\alpha^2 + 1)(\gamma^* - 1)/\tilde{\lambda}$. We find

$$\frac{\gamma - 1}{\lambda^*} \to \frac{1}{1-\gamma} \geq 1.$$ 

\[\square\]

### C.3 Analysis of the Main Equation

In this section we study the main equation of Theorem 1. Let,

$$P(f) = \sum_{j=1}^{K} \frac{\gamma_j}{\gamma} \int \left( \frac{\lambda_j}{t} + \frac{1}{1+\gamma f} \right)^{-1} dH_j(t),$$

then we are trying to solve $P(f) = f$. Numerically, this problem can be solved by bisection. Alternatively, a fixed point algorithm can be used to find $f$, as we now explain. These algorithms also prove constructively that $P(f) = f$ indeed has a root.

We first consider the case $\gamma < 1$ separately. Then we initialize $f$ arbitrarily, say $f_0 = 0$ and iteratively set $f_{m+1} = P(f_m)$ until convergence. If , then observe that for $f \geq 0$

$$P'(f) = \sum_{j=1}^{K} \frac{\gamma_j}{\gamma} \int \left( \frac{\lambda_j}{t} + \frac{1}{1+\gamma f} \right)^{-2} (1+\gamma f)^{-2} dH_j(t) \leq \gamma \sum_{j=1}^{K} \frac{\gamma_j}{\gamma} \int dH_j(t) = \gamma < 1.$$ 

We conclude that for $\gamma < 1$ the function $P$ is a contraction. As a result, the fixed point algorithm converges to the unique solution in $[0, \infty)$ and in fact

$$|f_m - f| = \mathcal{O}(\gamma^m).$$

Next, we consider a general $\gamma$. We define $u = \frac{1}{1+\gamma^*_T}$. Then,

$$\frac{1}{u} = 1 + \sum_{j=1}^{K} \gamma_j \int \left( \frac{\lambda_j}{t} + u \right)^{-1} dH_j(t) \implies 1 = u + \sum_{j=1}^{K} \gamma_j \int \frac{u}{\frac{\lambda_j}{t} + u} dH_j(t).$$

The function on the right hand side of the equation is increasing in $u \geq 0$, starting at 0 and going to $\infty$ as $u \to \infty$. Thus, there exists a unique such $u^*$, hence a unique solution $f \geq 0$. In addition, we have

$$u = \frac{1}{1 + \sum_{j=K}^{K} \gamma_j \int \left( \frac{\lambda_j}{t} + u \right)^{-1} dH_j(t)} = G(u).$$

37
Observe that $G$ is increasing in $u \geq 0$. Thus, if we initialize $u_0$ arbitrarily and iteratively define $u_{m+1} = G(u_m)$. If $u_0 < u^*$, then we can prove inductively that $u_m < u_{m+1} < u^*$. To see why, we compute

$$
\frac{u_m}{u_{m+1}} = u_m + \sum_{j=1}^{K} \gamma_j \int \frac{u_m}{\lambda + u_m} dH_j(t) < 1.
$$

In addition, $u_{m+1} = G(u_m) < G(u^*) = u^*$. Similarly, if $u_0 > u^*$, then inductively we have $u_{m+1} > u_m > u^*$. As a consequence, the sequence of iterates $u_m$ converges in both cases, and by the uniqueness of the fixed point $u^*$ we have $u_m \to u^*$.

## D Proofs for Section 4

### D.1 Lemma 2

**Proof of Lemma 2.** We first prove (28) and then lower bound the smallest eigenvalue of the matrix $A$.

**Concentration:** Fix $\tilde{\lambda} \in (0, \infty)$. In our argument here we consider $\tilde{\lambda}_{\text{init}}$ as deterministic and equal to $\tilde{\lambda}$. We can extend the proof using an almost identical argument as, say, in the proof of Lemma 1.

Now, let $M_{g}$ be the $p_g \times p$ matrix that consists of the rows of $M$ that correspond to the group $g$. It is enough to prove the following three asymptotic results.

$$
\|M_{g} w\|^2 - \left( \sum_{h=1}^{K} \|M_{g} x_h\|^2 \frac{\sigma_h^2}{p_h} \right) \xrightarrow{a.s.} 0 \quad (41)
$$

$$
\|N_{g} \varepsilon\|^2 - \|N_{g} \varepsilon\|^2 \frac{\sigma^2}{n} \xrightarrow{a.s.} 0 \quad (42)
$$

$$
\mathbf{w}^T M_{g}^T N_{g} \varepsilon \sqrt{n} \xrightarrow{a.s.} 0 \quad (43)
$$

Let us start with the proof of (41). First note that

$$
\|M_{g} x_h\|_F \leq \|M\|_F \leq \sqrt{p} \|M\| \leq \sqrt{p} \|X^T X / n\| / \tilde{\lambda} = O(\sqrt{p}).
$$

Applying Lemma 4 for $q = (4 + \eta)/2$ to the quadratic form $\|M_{g} x_h \mathbf{w} x_h \sqrt{p_h} \|^2 / p_h$ we see that:

$$
\mathbb{E} \left[ \left| \|M_{g} x_h \mathbf{w} x_h \sqrt{p_h} \|^2 / p_h - \mathbb{E} \left[ \|M_{g} x_h \mathbf{w} x_h \|^2 \right] \right| \right] \geq c \left( \frac{p^q/2}{p_h} \right) = O \left( \frac{1}{\sqrt{p}} \right).
$$

Thus, an application of the Borel-Cantelli lemma yields that

$$
\|M_{g} x_h \mathbf{w} x_h \|^2 - \|M_{g} x_h \mathbf{w} x_h \|^2 \frac{\sigma_h^2}{p_h} \xrightarrow{a.s.} 0.
$$

This implies (41). The derivation of (42) is analogous. Furthermore, also from Lemma 4 for $q = (4 + \eta)/2$ there exists a constant $C = C(q, \alpha_1, \ldots, \alpha_K, \sigma)$

$$
\left\| \mathbf{w}^T M_{g}^T N_{g} \frac{\varepsilon}{\sqrt{n}} \right\| \leq C \left( \frac{M_{g}^T N_{g} \frac{\varepsilon}{\sqrt{n}}}{\sqrt{p}} \right) \leq C \left( \frac{M_{g}^T N_{g} \varepsilon}{\sqrt{n}} \right) \leq O \left( \frac{1}{\sqrt{n}} \right),
$$

since $\|M_{g}^T \| \leq 1$ and $N_{g} \varepsilon = O(1)$. Another application of the Borel-Cantelli lemma proves (43).
We now sketch the argument using a leave-one-out technique. Recall that $z$ is bounded away from 0. Analogously, let $C_{i}$ the matrix given by taking the square of $n^{-1}X^{\top}X$ entrywise. We first observe that the $K \times K$ matrix $A$ is formed by taking the sum of entries in submatrices of $M_{i}$ divided by $n$. By analogy, we also define $B$ as the $K \times K$ matrix whose $(k, l)$--th entry is given by the sum of squares of entries in the $p_{k} \times p_{l}$ submatrix of $C_{i}$ divided by $n$.

Now consider the eigendecomposition $n^{-1}X^{\top}X = \sum_{i=1}^{p}d_{i}V_{i}^{\top}$. Then, the same eigenvectors diagonalize $M$ and

$$M = \sum_{i=1}^{p}d_{i}V_{i}^{\top}, \quad \tilde{d}_{i} = d_{i}/(d_{i} + \tilde{\lambda})$$

Let us also write $V_{ki}$ for the $i$--th coordinate of $V_{k}$ and let $a = (a_{1}, \cdots, a_{p})^{\top}$ be an arbitrary vector. It holds that $M_{ij} = \sum_{k=1}^{p}\tilde{d}_{k}V_{ki}V_{kj}$ and so:

$$a^{\top}M_{i}a = \sum_{i,j=1}^{p}a_{i}a_{j}M_{ij}^{2}$$

$$= \sum_{i,j=1}^{p}a_{i}a_{j}d_{k}d_{l}V_{ki}V_{kj}V_{li}V_{lj}$$

$$= \sum_{i,j=1}^{p}\tilde{d}_{k}\tilde{d}_{l}\left(\sum_{i=1}^{p}a_{i}V_{ki}V_{li}\right)^{2}$$

$$\geq \frac{1}{(d_{1} + \tilde{\lambda})^{2}}\sum_{i,j=1}^{p}d_{k}d_{l}\left(\sum_{i=1}^{p}a_{i}V_{ki}V_{li}\right)^{2}$$

$$= \frac{a^{\top}C_{i}a}{(d_{1} + \tilde{\lambda})^{2}}.$$  \hspace{1cm} (44)

Now given any $K$-dimensional vector $\tilde{a}$, we can expand it as $a$ with $a_{i} = a_{j} = \tilde{a}_{g}$ for all $i, j \in G_{g}$ and $g = 1, \ldots, K$, which yields:

$$\tilde{a}^{\top}A\tilde{a} \geq \frac{\tilde{a}^{\top}B\tilde{a}}{(d_{1} + \tilde{\lambda})^{2}}.$$  \hspace{1cm} (45)

Since $d_{1}$ is uniformly bounded almost surely, we conclude that, in order to show that the smallest eigenvalue of $A$ is bounded away from zero, it suffices to show that the smallest eigenvalue of $B$ is bounded away from 0.

Using Lemma 4 we can show that for any matrices $A_{1}, A_{2}$ bounded in operator norm

$$\frac{\text{Tr} \left( A_{1}Z_{n}^{\top}A_{2}Z_{n} \right)}{n} - \frac{\gamma^{2}\text{Tr} \left( A_{1}A_{2} \right)}{n} - \frac{\gamma \text{Tr} \left( A_{1} \right) \text{Tr} \left( A_{2} \right)}{n} \overset{a.s.}{\rightarrow} 0.$$  \hspace{1cm} (46)

We now sketch the argument using a leave-one-out technique. Recall that $z_{i}$ is the $i$--th row of $Z$ and let $Z_{i}$ the matrix that we get if we delete that row from $Z$, then

$$\frac{\text{Tr} \left( A_{1}Z_{n}^{\top}A_{2}Z_{n} \right)}{n} = \frac{\sum_{i=1}^{p}z_{i}^{\top}A_{1} \left( \frac{Z_{i}^{\top}Z_{i}}{n} + \frac{z_{i}z_{i}^{\top}}{n} \right) A_{2}z_{i}}{n^{2}}$$

$$\quad \quad \quad = \sum_{i=1}^{p}z_{i}^{\top}A_{1}z_{i}z_{i}^{\top}A_{2}z_{i}/n + \sum_{i=1}^{p}z_{i}^{\top}A_{1}Z_{i}^{\top}A_{2}Z_{i}/n$$

$$39$$
With Lemma 4 and Borel Cantelli we can show that almost surely (and uniformly in \(i\))

\[
\frac{1}{n} \sum_{i=1}^{p} z_i^T A_1 Z_i n A_2 z_i / n = \frac{p}{n} \left\{ n^{-1} \text{Tr} \left( A_1 \frac{Z_i Z_i}{n} A_2 \right) \right\} + o(1),
\]

and that

\[
n^{-1} \text{Tr} \left( A_1 \frac{Z_i Z_i}{n} A_2 \right) = \frac{\text{Tr}(A_1 A_2)}{n} + o(1),
\]

By the same reasoning

\[
\frac{1}{n} \sum_{i=1}^{p} z_i^T A_1 z_i z_i^T A_2 z_i = \frac{p}{n} \left\{ \frac{\text{Tr}(A_1)}{n} \frac{\text{Tr}(A_2)}{n} \right\} + o(1).
\]

Now let \( \Sigma_{g_k, g_{\ell i}} \in \mathbb{R}^{p \times p} \) be the submatrix of \( \Sigma \) that corresponds to the covariance of the \( k \)-th and \( \ell \)-th groups and also let \( R_k \in \mathbb{R}^{p \times p} \) the submatrix of \( \Sigma^{1/2} \) consisting of the columns that correspond to the \( k \)-th group. Then, as a result of (46) the \((k, \ell)\)-th entry of \( B \) is given by

\[
\frac{\text{Tr} \left( R_k^T \Sigma_{g_k, g_{\ell i}} R_{k} \right)}{n} = \gamma^2 \frac{\text{Tr}(R_k R_k^T)}{n} + \gamma^2 \frac{\text{Tr}(R_k R_k^T R_{k} R_{\ell}^T)}{n} + o(1)
\]

and so

\[
B = \gamma \text{tr} \left( \frac{\Sigma_{g_k, g_{\ell i}}}{n} \right) + \gamma^2 \left( n^{-1} \text{tr} \left( \Sigma_{g_k, g_{\ell i}} \right) \right)_{1 \leq k, \ell \leq K} + o(1),
\]

which has eigenvalues uniformly bounded away from 0. To see why, we revisit the key idea of the argument from (44). Let \( \Sigma_s \) be the \( p \times p \) matrix with \((i, j)\)-th entry equal to \( \Sigma_{ij}^2 \). Also let \( \Sigma \) be the \( K \times K \) matrix with \((k, \ell)\)-entry \( \Sigma_{k\ell} = n^{-1} \| \Sigma_{g_k, g_{\ell i}} \|_F^2 \). Now let \( \Sigma = \sum_{i=1}^{p} d_i V_i V_i^T \) the spectral decomposition of \( \Sigma \) (with some abuse of notation; this spectral decomposition is not the same as the one of \( X^T X / n \)). Next let \( a = (a_1, \ldots, a_p) \in \mathbb{R}^p \) arbitrary and \( d_{\min} \) the smallest eigenvalue of \( \Sigma \) and observe that:

\[
a^T \Sigma_s a = \sum_{i,j=1}^{p} a_i a_j \Sigma_{ij}^2
\]

\[
= \sum_{i,j=1}^{p} a_i a_j \sum_{k, \ell=1}^{p} d_k d_{\ell} V_{ki} V_{\ell i} V_{ki} V_{\ell j}
\]

\[
\geq d_{\min} \sum_{k, \ell=1}^{p} \left( \sum_{i=1}^{p} a_i V_{ki} V_{\ell i} \right)^2
\]

\[
= d_{\min} \| a \|_2^2
\]
Fix \( \tilde{a} \in \mathbb{R}^K \) and expand it as \( a \) with \( a_i = a_j = \tilde{a}_g \) for all \( i, j \in G_g \) and \( g = 1, \ldots, K \), then:

\[
\tilde{a}^\top \Sigma \tilde{a} = n^{-1} a^\top \Sigma a \\
\geq n^{-1} d_{\min} \|a\|_2^2 \\
\geq n^{-1} d_{\min} \sum_{k=1}^K p_k \tilde{a}_k^2 \tag{48}
\]

\[\geq \min_{k=1,\ldots,K} \left\{ \frac{p_k}{n} \right\} \cdot d_{\min} \cdot \|a\|_2^2 \]

\[\square\]

### D.2 Lemma 3

**Proof of Lemma 3.** For the proof of this lemma we assume without loss of generality that \( \sigma = 1 \).

For the leave-one-out cross-validation risk we have the famous shortcut formula (which can be found, for example, in Hastie et al. [2019])

\[
CV_n^*(\lambda) = \frac{1}{n} \sum_{i=1}^n \left( \frac{y_i - x_i^\top \hat{w}(\lambda)}{1 - (S_{\lambda})_{ii}} \right)^2,
\]

where \( S_{\lambda} = \frac{1}{n} X \left( \frac{X^\top X}{n} + \Lambda \right)^{-1} X^\top \) is the group-regularized ridge regression smoother matrix. We will use the notation

\[M = \left( \frac{Z^\top Z}{n} + \Sigma^{-\frac{1}{2}} \Lambda \Sigma^{-\frac{1}{2}} \right)^{-1}.
\]

We divide the proof into three main steps.

1. We show that for any \( \Lambda \) the denominators approach \( 1/(1 + n^{-1} \text{Tr}(M)) \).

2. We find asymptotic approximations for the sums of the numerators to complete the proof of pointwise convergence.

3. We control \( \nabla_\lambda CV_n^*(\lambda) \) to prove that convergence is uniform on compact subsets of \((0, \infty)^K\).

**Step 1:** It is convenient to first note that \( (S_{\lambda})_{ii} = \frac{z_i^\top M z_i}{n} \). Next let

\[M_i = \left( \frac{Z^\top Z}{n} + \Sigma^{-\frac{1}{2}} \Lambda \Sigma^{-\frac{1}{2}} - \frac{z_i z_i^\top}{n} \right)^{-1}.
\]

We have the resolvent identity

\[M^{-1} = M_i^{-1} + n^{-1} z_i z_i^\top \implies M_i = M + M_i \frac{z_i z_i^\top}{n} M \implies \frac{z_i^\top M z_i}{n} = \frac{z_i^\top M_i z_i}{1 + \frac{z_i^\top M_i z_i}{n}} \tag{49}
\]

Using Lemma 4 (upon conditioning on \( M_i \)), the union bound and Borel-Cantelli we have that

\[\max_i \left| \frac{z_i^\top M_i z_i}{n} - n^{-1} \text{Tr}(M_i) \right| \xrightarrow{a.s.} 0. \tag{50}
\]
Now we prove that $n^{-1} \text{Tr}(M_i)$ is close to $n^{-1} \text{Tr}(M)$, i.e. that

$$\max_i n^{-1} |\text{Tr}(M_i) - \text{Tr}(M)| \overset{a.s.}\to 0. \quad (51)$$

To see this, first note that $M^{-1} \succeq M_i^{-1} \succeq \Sigma^{-1/2} \Lambda \Sigma^{1/2}$, i.e., $M \preceq M_i \preceq \Sigma^{-1/2} \Lambda^{-1} \Sigma^{1/2}$, and so $M, M_i$ have uniformly bounded eigenvalues. Second, $M_i - M = M_i \frac{z_i z_i^T}{n}$ has rank 1. These results together imply that

$$0 \leq \text{Tr}(M_i) - \text{Tr}(M) \leq \|M_i - M\| = O(1)$$

almost surely and uniformly in $i, n$ for any fixed $\Lambda$, hence (51) follows. Combining (50) and (51) we see that

$$\max_i \left| \frac{z_i^T M_i z_i}{n} - n^{-1} \text{Tr}(M) \right| \overset{a.s.}\to 0,$$

Replacing the quadratic forms in (49) by the normalized trace of $M$ (which is uniformly bounded) we get

$$\max_i \left| (S_{\Lambda})_{ii} - \frac{n^{-1} \text{Tr}(M)}{1 + n^{-1} \text{Tr}(M)} \right| \overset{a.s.}\to 0 \quad (52)$$

Step 2: The average of the numerators in the shortcut formula for the leave-one-out cross-validation error is

$$\frac{\|Y - X \hat{w}(\Lambda)\|^2}{n} = \frac{1}{n} \left\| X w + \varepsilon - X \left( \frac{X^T X}{n} + \Lambda \right)^{-1} \left( \frac{X^T X w + X^T \varepsilon}{n} \right) \right\|^2$$

$$= \frac{1}{n} \left\| X \left( \frac{X^T X}{n} + \Lambda \right)^{-1} \Lambda w + \left( I_n - \frac{1}{n} X \left( \frac{X^T X}{n} + \Lambda \right)^{-1} X^T \right) \varepsilon \right\|^2,$$

which, by the same concentration argument as we did for the out-of-sample error in Lemma 1, is asymptotically approximated almost surely by

$$\frac{1}{n} \left\| \left( I_n - \frac{1}{n} X \left( \frac{X^T X}{n} + \Lambda \right)^{-1} X^T \right) \right\|_F^2 + \frac{1}{p} \text{Tr} \left( \left( \frac{X^T X}{n} + \Lambda \right)^{-1} \frac{X^T X}{n} \Lambda^{-1} \Lambda \hat{D} \Lambda \right). \quad (53)$$

Firstly we provide asymptotics for the first term in (53). It is equal to

$$E_1 = 1 - \frac{2}{n} \text{Tr} \left( \left( \frac{X^T X}{n} + \Lambda \right)^{-1} \frac{X^T X}{n} \right) \right\|_F^2 + \frac{1}{p} \text{Tr} \left( \left( \frac{X^T X}{n} + \Lambda \right)^{-1} \frac{X^T X}{n} \right), \quad (54)$$

We see that

$$\frac{1}{n} \text{Tr} \left( \left( \frac{M Z^T Z}{n} \right)^2 \right) = \frac{1}{n} \sum_{1 \leq i, j \leq n} \left( \frac{z_i^T M z_j}{n^2} \right)^2, \quad (55)$$
where the terms for \(i = j\) are just the diagonal entries of \(S\) squared. Hence, by (52) it follows that the average of those terms gives asymptotically \((\frac{1}{n} \text{Tr}(S))^2\), so from (54) and (55) we see that

\[
E_1 = \left(1 - \frac{1}{n} \text{Tr}(S)\right)^2 + \frac{1}{n} \sum_{i \neq j} \frac{(z_i^T M z_j)^2}{n^2} + o(1)
\]

Using again the resolvent identity \(M_i = M + M_i \frac{z_i^T}{n} M\) we deduce that

\[
z_i^T M z_i = \frac{z_i^T M_i z_i}{1 + z_i^T M_i z_i},
\]

and so that

\[
\frac{1}{n} \sum_{i} \sum_{j \neq i} \frac{(z_i^T M z_j)^2}{n^2} = \frac{1}{n} \sum_{i} \frac{(1 + \frac{z_i^T M_i z_i}{n})^{-2}}{n} z_i^T M_i \left(\sum_{j \neq i} \frac{z_j^T}{n}\right) M_i z_i
\]

\[
= \left(1 + o(1)\right) \frac{(1 + n^{-1} \text{Tr}(M))^{-2}}{n} \sum_{i} \frac{1}{n} z_i^T M_i \left(\sum_{j \neq i} \frac{z_j^T}{n}\right) M_i z_i
\]

At this point we observe that by Lemma 4 and Borel-Cantelli we have:

\[
\max_i \frac{1}{n} \left| z_i^T M_i \left(\sum_{j \neq i} \frac{z_j^T}{n}\right) M_i z_i - \text{Tr} \left( M_i^2 \sum_{j \neq i} \frac{z_j^T z_j}{n} \right) \right| \xrightarrow{a.s.} 0.
\]

Here we also used the fact that \(\sum_{j \neq i} z_j z_j^T / n \preceq Z^T Z / n\). Next we will need the following lemma, which we are going to prove after the end of this proof.

**Lemma 5.** With the assumptions we made it holds that:

\[
\max_i \frac{1}{n} \left| \text{Tr} \left( M_i^2 \sum_{j \neq i} \frac{z_j z_j^T}{n} \right) - \text{Tr} \left( M_i^2 \frac{Z^T Z}{n} \right) \right| \xrightarrow{a.s.} 0.
\]

Combining Lemma 5 and (59) we conclude that

\[
\max_i \frac{1}{n} \left| z_i^T M_i \left(\sum_{j \neq i} \frac{z_j^T}{n}\right) M_i z_i - \text{Tr} \left( M_i^2 \frac{Z^T Z}{n} \right) \right| \xrightarrow{a.s.} 0.
\]

Finally, combining (56) and (61) we have proved that

\[
E_1 = \left(1 - \frac{\text{Tr}(S)}{n}\right)^2 + \frac{n^{-1} \text{Tr}(M^2 \frac{Z^T Z}{n})}{(1 + n^{-1} \text{Tr}(M))^2} + o(1)
\]

\[
= (1 + n^{-1} \text{Tr}(M))^{-2} \left(1 + n^{-1} \text{Tr}(M^2 \frac{Z^T Z}{n})\right) + o(1)
\]

Now it is time to examine the second term of (53). Let \(\overline{\Sigma} = \Sigma^{-\frac{1}{2}} \Lambda \overline{\Delta} \Lambda \Sigma^{-\frac{1}{2}}\). The second term of
(53) equals
\[ E_2 = p^{-1} \text{Tr} \left( \left( \frac{X^\top X}{n} + \Lambda \right)^{-1} \frac{X^\top X}{n} \left( \frac{X^\top X}{n} + \Lambda \right)^{-1} \Lambda \bar{D} \Lambda \right) \]
\[ = \frac{1}{p} \text{Tr} \left( M \frac{Z^\top M \Sigma}{n} M \Sigma \right) \]
\[ = \frac{1}{p} \sum_{i=1}^{n} \frac{z_i^\top M \Sigma M z_i}{n} \] (63)

Using the resolvent identity \( M_i = M + \frac{M z_i z_i^\top M}{n} \) we derive
\[ M z_i = \left( 1 - \frac{z_i^\top M z_i}{n} \right) \frac{M z_i}{1 + \frac{z_i^\top M z_i}{n}}. \] (64)

Replacing this in (63) we get:
\[ E_2 = \frac{1}{p} \sum_{i=1}^{n} \left( 1 - (S \Lambda)_{ii} \right) \frac{z_i^\top M \Sigma M z_i}{n} \] (65)

In the same way as we proved (61) we can prove that
\[ \max_i \left| \frac{z_i^\top M \Sigma M z_i}{n} - \frac{1}{p} \text{Tr}(M^2 \Sigma) \right| \overset{\text{a.s.}}{\longrightarrow} 0 \] (66)

Combining (52) and (66) we get:
\[ E_2 = \frac{\left( (1 + n^{-1} \text{Tr}(M))^2 \right)^{-2}}{p} \text{Tr}(M^2 \Sigma) + o(1). \] (67)

Using (52), (62) and (67) we have:
\[ CV_n^*(\lambda) = 1 + \frac{1}{n} \text{Tr} \left( M^2 \frac{Z^\top Z}{n} \right) + \frac{1}{p} \text{Tr} \left( M^2 \Sigma^{-\frac{1}{2}} \Lambda \bar{D} \Lambda \Sigma^{-\frac{1}{2}} \right) + o(1) \] (68)

Omitting the \( o(1) \), this is exactly the expression of \( L_n(\lambda) \).

**Step 3:** For \( \lambda \) taking values in a compact set \( C \) of \((0, \infty)^K\) we have that the functions \( CV_n^*(\lambda) \), as we can see by using the shortcut formula, are almost surely uniformly bounded and uniformly Lipschitz, hence uniformly equicontinuous. The same holds for \( L_n \), so also for the difference \( CV_n^* - L_n \). By the pointwise convergence that we showed in the second step we have that almost surely in a countable dense subset \( C_d \) of \( K \) we have \( CV_n^* - L_n \overset{\text{a.s.}}{\longrightarrow} 0 \). Since by the Arzela-Ascoli theorem almost surely any subsequence of \( \{ CV_n^* - L_n \}_{n \geq 1} \) has a uniformly convergent subsequence and since by pointwise convergence on \( C_d \) the only uniform subsequential limit can be 0, we know that
\[ \sup_{\lambda \in C} |CV_n^*(\lambda) - L_n(\lambda)| \overset{\text{a.s.}}{\longrightarrow} 0. \]

The proof is completed.

**Proof of Lemma 5.** Let \( R = \Sigma^{-\frac{1}{2}} \Lambda \Sigma^{-\frac{1}{2}} \). We have
\[ \frac{1}{n} \text{Tr}(M_i^2 \sum_{j \neq i} \frac{z_j z_j^\top}{n}) = n^{-1} \text{Tr} \left( M_i^2 (M_i^{-1} - R) \right) = \frac{\text{Tr}(M_i) - \text{tr}(M_i^2 R)}{n} \]

44
and
\[
\frac{1}{n} \text{Tr}(M^2 \sum_j \frac{z_j z_j^T}{n}) = n^{-1} \text{Tr}(M^2(M^{-1} - R)) = \frac{\text{Tr}(M) - \text{Tr}(M^2R)}{n}.
\]

In light of (51), it suffices to show that
\[
\max_i \left| \frac{\text{Tr}((M_i^2 - M^2)R)}{n} \right| \overset{a.s.}{\to} 0.
\]

We have that \(M_i^2 - M^2 = M_i^2 \left(M^{-2} - M_i^{-2}\right) M^2\) has rank at most 2 (by expanding the middle terms), so by the fact that \(M_i^2, M^2, R\) have uniformly bounded operator norm, it follows that almost surely
\[
\max_i \left| \frac{\text{Tr}((M_i^2 - M^2)R)}{n} \right| = O(n^{-1}).
\]

This completes the proof of the lemma. \(\Box\)

D.3 Theorem 2

Proof of Theorem 2. It only remains to extend the argument to noncompact sets. We fix \(M > 0\) large and consider for each \(\lambda \in V_2\) the matrix \(\Lambda_{M}\) that we get by truncating entries of \(\Lambda\) that are larger than \(M\) to \(M\). Let \(\hat{w}(\Lambda)\) be the estimator of \(w\) using ridge regression with penalty matrix \(\Lambda\) and \(\hat{w}(\Lambda_{M})\) the estimator using the penalty matrix \(\Lambda_{M}\). We first check that it suffices to show that
\[
\lim_{M \to \infty} \lim_{n \to \infty} \sup_{\Lambda \in V_2} \|\hat{w}(\Lambda_{M}) - \hat{w}(\Lambda)\| = 0 \text{ almost surely.} \tag{69}
\]

To see that the above suffices, note that we can write
\[
R(\hat{w}(\Lambda_{M})) - R(\hat{w}(\Lambda)) = (\hat{w}(\Lambda_{M}) - w)^T \Sigma (\hat{w}(\Lambda_{M}) - w) - (\hat{w}(\Lambda) - w)^T \Sigma (\hat{w}(\Lambda) - w)
\]
\[
= \hat{w}(\Lambda_{M})^T \Sigma \hat{w}(\Lambda_{M}) - \hat{w}(\Lambda)^T \Sigma \hat{w}(\Lambda) - 2w^T \Sigma (\hat{w}(\Lambda_{M}) - \hat{w}(\Lambda))
\]
\[
= (\hat{w}(\Lambda_{M}) - \hat{w}(\Lambda))^T \Sigma \hat{w}(\Lambda_{M}) + \hat{w}(\Lambda)^T \Sigma (\hat{w}(\Lambda_{M}) - \hat{w}(\Lambda)) - 2w^T \Sigma (\hat{w}(\Lambda_{M}) - \hat{w}(\Lambda)).
\]

We can show that \(\|\Sigma \hat{w}(\Lambda_{M})\|_2, \|\Sigma \hat{w}(\Lambda)\|_2, \|\Sigma w\|_2\) are bounded uniformly in \(n\) and \(\Lambda\) almost surely, and so (69) implies that
\[
\lim_{M \to \infty} \lim_{n \to \infty} \sup_{\Lambda \in V_2} |R(\hat{w}(\Lambda_{M})) - R(\hat{w}(\Lambda))| = 0 \text{ almost surely.} \tag{70}
\]

It remains to prove (69). We temporarily fix \(\Lambda\). We also let \(S_1 = (n^{-1}X^TX + \Lambda)^{-1}\), \(S_2 = (n^{-1}X^TX + \Lambda_{M})^{-1}\). Next, assume without loss of generality that only the last \(j\) groups have \(\lambda_g\) exceeding \(M\), and let \(\Lambda_1, \Lambda_2\) be the diagonal submatrices of \(\Lambda\) that correspond to the first \(K - j\) and last \(j\) groups respectively, and write
\[
\frac{X^TX}{n} = \begin{pmatrix} \Lambda_1 & S_{12} \\ S_{21} & \Lambda_2 \end{pmatrix},
\]

where \(S_{22}\) is the sample covariance of the features in the last \(j\) groups. Then:
\[
S_1 = \begin{pmatrix} \Lambda_1 + S_{12} (S_{22} + \Lambda_2)^{-1} S_{21} \\ \ast \end{pmatrix}^{-1} - \begin{pmatrix} \Lambda_1 - S_{12} (S_{22} + \Lambda_2)^{-1} S_{21} \\ \ast \end{pmatrix}^{-1} S_{12} (S_{22} + \Lambda_2)^{-1},
\]

45
where * is completed to make $S_1$ symmetric. We also note that $S_{11}, S_{12}, S_{22}$ are bounded in operator norm due to the fact that:
\[
\max \{ \|S_{11}\|, \|S_{12}\|, \|S_{22}\| \} \leq \|S\| = n^{-1} \|X\|^2.
\]
Thus, uniformly in $\Lambda_1$ we have:
\[
S_1 = \left( (S_{11} + \Lambda_1)^{-1} 0 0 \right) + O_{\text{op}}(M^{-1}).
\]
The same argument holds for $S_2$ and we get $\|S_1 - S_2\| = O(M^{-1})$ in operator norm. It follows that
\[
\|\hat{w}(\Lambda_M) - \hat{w}(\Lambda)\| = \left\| (S_1 - S_2) \frac{X^\top Y}{n} \right\| \leq \|S_1 - S_2\| \left\| \frac{X}{\sqrt{n}} \right\| \left\| \frac{Y}{\sqrt{n}} \right\| = O(M^{-1}),
\]
where we have used the fact that $\limsup (n^{-1/2} \|X\| \leq \limsup \|\Sigma\|^{1/2} n^{-1/2} \|Z\| = (1 + \sqrt{\gamma}) \|\Sigma\|^{1/2}$.

### D.4 Corollary 5

**Proof of Corollary 5.** It is enough to show that any set of coefficients that can be achieved using Group Lasso can also be achieved by suitably choosing the parameters of Group Ridge. Let $\lambda'_g = \lambda_{1}^g \sqrt{p_i/p}, \ldots, \lambda'_K = \lambda_{K}^g \sqrt{p_K/p}$ be the parameters of Group Lasso, giving weights $\tilde{w}_g \in \mathbb{R}^{p_g}, 1 \leq g \leq K$ for the groups respectively. Let $\lambda_g = \lambda'_g / \|\tilde{w}_{G_g}\|$ be the group ridge parameters for the corresponding ridge regression and write $\lambda = (\lambda_1, \ldots, \lambda_K)$. We claim that the group-ridge solution $\hat{w}(\lambda)$ from (2) is equal to $\tilde{w}$. First notice that if for a group it holds that $\tilde{w}_g = 0$, then $\lambda_g = \infty$, and so Ridge will also assign $\hat{w}_g(\lambda) = 0$. Upon removing the subset of groups $g$ such that $\tilde{w}_g \neq 0$ from the design matrix $X$, we may assume without loss of generality that all $\tilde{w}_g \neq 0$ and so all $\lambda_i \in (0, \infty)$. Then,
\[
\nabla_w \left( \frac{\|Y - Xw\|^2}{2n} + \sum_{i=1}^K \lambda_g \|\tilde{w}_{G_g}\|^2 \right) \bigg|_{w = \tilde{w}} = \frac{X^\top (X \tilde{w} - Y)}{n} + \sum_{g=1}^K \frac{\lambda'_g}{\|\tilde{w}_{G_g}\|} \tilde{w}_{G_g} = 0,
\]
since the last expression is exactly the gradient of the Group Lasso loss evaluated at the minimizer $\tilde{w}$.

The conclusion follows by an application of Theorem 2. To apply the theorem we need to argue that $\lambda_g$ are bounded away from 0 for large $n$ almost surely. It suffices to show that $\|\tilde{w}_g\|_2$ is bounded away from infinity. By comparing the objective value of the Group Lasso at $\tilde{w}$ and at 0, we see that for all $g$,
\[
\lambda'_g \cdot \|\tilde{w}_g\|_2 \leq \frac{1}{2n} \|Y\|_2^2
\]
By our assumptions, the RHS is bounded almost surely. The LHS satisfies (deterministically)
\[
\liminf_{n \to \infty} \lambda'_g \geq \sqrt{\gamma} \cdot \delta > 0
\]
and so we conclude. \qed
E Additional figures

Figure S1: Asymptotic predictions for asymptotic risk of group-regularized ridge regression. This figure is analogous to Figure 4 with a different feature covariance. $\Sigma_1 = \Sigma_2$ have eigenvalues equal to the evenly-spaced quantiles of the Exponential distribution with rate 0.5.