On the Degrees of Freedom of some Lasso procedures

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Abstract

The effective degrees of freedom of penalized regression models quantify the actual amount of information used to generate predictions, playing a pivotal role in model evaluation and selection. Although a closed-form estimator is available for the Lasso penalty, adaptive extensions of widely used penalized approaches, including the Adaptive Lasso and Adaptive Group Lasso, have remained without analogous theoretical characterization. This paper presents the first unbiased estimator of the effective degrees of freedom for these methods, along with their main theoretical properties, for both orthogonal and non-orthogonal designs, derived within Stein's unbiased risk estimation framework. The resulting expressions feature inflation terms influenced by the regularization parameter, coefficient signs, and least-squares estimates. These advances enable more accurate model selection criteria and unbiased prediction error estimates, illustrated through synthetic and real data. These contributions offer a rigorous theoretical foundation for understanding model complexity in adaptive regression, bridging a critical gap between theory and practice.

Keywords: Degrees of Freedom; Adaptive Lasso; Stein's Lemma.

1 Introduction

Regularization has become a cornerstone of modern statistical modeling, particularly in regression settings where estimators are defined by minimizing an objective function comprising a loss term and a penalty on coefficient norms. Among such methods, the Lasso estimator (Tibshirani, 1996), which employs the ℓ_1 norm, achieves variable selection by shrinking a subset of coefficients exactly to zero, thereby inducing sparsity. Extensions such as the Group Lasso (Yuan and Lin, 2006) generalize this framework to structured settings, applying ℓ_2 penalties to predefined groups of coefficients to enable group-wise selection. While these methods excel at regularization, their uniform shrinkage mechanisms lead to over shrink also the signal, thus producing biased estimates of the non zero coefficients. The Adaptive Lasso (Zou, 2006) and its extensions address this limitation by incorporating data-driven weights derived from preliminary least squares estimates. Unlike its non-adaptive counterpart, which imposes uniform shrinkage, the Adaptive Lasso adapts penalization to individual coefficients, reducing bias and attaining oracle properties under suitable conditions. Similarly, the Adaptive Group Lasso (Wang and

Leng, 2008), combines group-structured regularization with coefficient-specific adaptation. A central concept in statistical modeling is the notion of degrees of freedom. For example, in a normal linear regression framework, let $\mathbf{X}$ be a matrix of covariates with p columns, $\mathbf{y}$ be the response vector of size n, and $\boldsymbol{\beta}$ the p-dimensional vector of unknown regression coefficients with $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$ and $\boldsymbol{\epsilon} \sim \mathrm{N}(\mathbf{0}, \sigma^2 \mathbf{I}_n)$. In these settings, the degrees of freedom can be thought as the number of "independent pieces of information" needed to estimate the p unknown parameters. For simple least-squares estimates of $\boldsymbol{\beta}$ the degrees of freedom equal the number of variables p implying that each estimated quantity "consumes" one degree of freedom. A general notion of degrees of freedom is given by Efron (1986) as follows

$$df(\widehat{\mathbf{y}}) = \frac{1}{\sigma^2} \sum_{i=1}^{n} \mathbb{C}\mathrm{ov}(y_i, \widehat{y}_i), \tag{1}$$

where $\widehat{\mathbf{y}} = (\widehat{y}_1, \ldots, \widehat{y}_n)$ is the vector of predictions obtained from the model under consideration and σ^2 is the (unknown) variance of the response. Notably, both $\mathbf{y}$ and $\widehat{\mathbf{y}}$ need to be considered as random quantities. In practice Equation (1) says that the more the predictions of the model are near to observed values, the higher the degrees of freedom. This notion of similarity can be written also in term of divergence, leading to the celebrated Stein's Lemma (Stein, 1981):

$$df(\widehat{\mathbf{y}}) = \mathbb{E}(\nabla \widehat{\mathbf{y}}) = \mathbb{E}\left[\mathrm{trace}\left(\frac{\partial \widehat{\mathbf{y}}}{\partial \mathbf{y}}\right)\right]. \tag{2}$$

Under these settings, Zou et al. (2007) proved that an unbiased estimate of the degrees of freedom of Lasso regression is the number of nonzero coefficients estimated by the model, often referred as the size of the *active set*. This can be surprising, since differently from (random) subset regression, Lasso selects nonzero coefficients using the response variable so one would expect a higher value for the degrees of freedom. Nevertheless, this additional use of data is perfectly balanced with the amount of shrinkage that Lasso applies to each coefficient. Note that this would not happen in subset selection, where the "best" subset of variables to use in a linear model is chosen accordingly to some criteria (see Tibshirani, 2015). Similar results were found for the generalized Lasso penalty (Tibshirani and Taylor, 2011; Chen et al., 2020) and for the more challenging case $p > n$ (Dossal et al., 2013; Tibshirani and Taylor, 2012). This perfect trade-off between shrinkage and the use of the response variable does not arise for the Group Lasso estimator, as discussed by Vaiter et al. (2017). In this work, the authors derive formulae for computing the degrees of freedom of the Group Lasso under both orthogonal and non-orthogonal designs, generally yielding values lower than the size of the active set (see also Vaiter et al., 2012). The concept of degrees of freedom underpins parametric inference and model selection: information criteria such as the Akaike Information Criterion (AIC) and Bayesian Information Criterion (BIC) are defined by combining a model fit measure and the degrees of freedom (Säfken et al., 2024). Despite their advantages, adaptive methods lack a closed-form expression for their effective degrees of freedom. While such estimators exist for non-adaptive methods like the Lasso (Zou et al., 2007), adaptive variants resist analogous characterization due to their data-dependent weights, which introduce nonlinear dependencies between coefficients and penalties. Furthermore, the simplicity of the degrees of freedom formula for the Lasso estimator has inadvertently encouraged the misguided practice of computing information criteria for arbitrary penalized methods by substituting the size of the active set for the true degrees of freedom. This flawed approach risks overly optimistic model selection, often leading to overfitting and biased parameter estimates. In this paper, we solve this issue by deriving the first unbiased estimator of the effective degrees of freedom for the Adaptive Lasso within Stein's unbiased risk estimation framework (Stein, 1981). Our estimator explicitly accounts for the adaptive penalty's dependence on data-driven weights, regularization parameters, and coefficient signs. The proof

of our main results follows similar arguments to those in Zou et al. (2007), which examined the first-order conditions of the Lasso optimization problem. However, in Adaptive Lasso and related models, an additional term appears that does not vanish. The explicit derivation of this term's gradient with respect to the data is obtained using matrix differentiation rules. Additionally, we re-derive the expression for the degrees of freedom of the Group Lasso, providing additional insights and characterizations by means of an application of the implicit function theorem, thus complementing Yuan and Lin (2006) and Vaiter et al. (2017). Leveraging these results, we are also able to provide analogous derivations for the more challenging Adaptive Group Lasso estimator. By bridging this theoretical gap, our work enables principled model selection, risk estimation, and complexity-aware inference for adaptive penalized regression methods.

1.1 Notation and organization of the paper

Throughout the paper, we assume a normal linear regression model $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$ with $\boldsymbol{\epsilon} \sim N(\mathbf{0}, \sigma^2\mathbf{I}_n)$, $\mathbf{X} \in \mathbb{R}^{n \times p}$, $\mathbf{y} \in \mathbb{R}^n$, and $\boldsymbol{\beta} \in \mathbb{R}^p$. We refer to the orthonormal design whenever $\mathbf{X}^\top\mathbf{X} = \mathbf{I}_p$ i.e., variables are uncorrelated and standardized. The least squares estimator of $\boldsymbol{\beta}$ is given by $\widehat{\boldsymbol{\beta}}^{\mathsf{LS}} = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}$. Let $\gamma \in \mathbb{R}_+$ denote the regularization parameter common to the penalized methods under study. For a fixed γ, we denote by $\widehat{\boldsymbol{\beta}}_\gamma$, $\widehat{\mathbf{y}}_\gamma$, and $\widehat{df}_\gamma$ the vector of estimated coefficients, the predictions, and the estimated degrees of freedom, respectively. When unambiguous, we may suppress the dependence on γ in the notation (e.g., $\widehat{\boldsymbol{\beta}}$ for $\widehat{\boldsymbol{\beta}}_\gamma$) to simplify exposition. The *transition points*, i.e. the values of γ for which the active set changes are denoted by γ_l with $l = 1, \ldots, L$ where L is the number of such points. Information criteria are defined as

$$AIC(\widehat{\mathbf{y}}_\gamma) = \frac{\|\mathbf{y} - \widehat{\mathbf{y}}_\gamma\|_2^2}{n\sigma^2} + \frac{2}{n}\widehat{df}_\gamma, \quad BIC(\widehat{\mathbf{y}}_\gamma) = \frac{\|\mathbf{y} - \widehat{\mathbf{y}}_\gamma\|_2^2}{n\sigma^2} + \frac{\log(n)}{n}\widehat{df}_\gamma. \tag{3}$$

The operator $|\cdot|$ denotes either the absolute value of a scalar, i.e., $|a|$ for $a \in \mathbb{R}$, or the cardinality of a set, i.e., $|\mathcal{A}|$ for a set $\mathcal{A}$. For a square matrix $\mathbf{M}$, diag($\mathbf{M}$) extracts the vector of its diagonal elements. For a vector $\mathbf{v} = (v_1, \ldots, v_p)^\top$, diag($\mathbf{v}$) constructs a diagonal matrix with entries $v_1, \ldots, v_p$. The operator trace($\cdot$) denotes the trace of a square matrix. The function sgn($\cdot$) denotes the sign of a scalar or a vector. The remainder of the paper is structured as follows. Section 2 presents our core theoretical contributions: closed-form expressions for the effective degrees of freedom in Adaptive Lasso, Group Lasso, and Adaptive Group Lasso, accompanied by interpretative remarks and complementary characterizations. Section 3 provides empirical validation of these results and illustration of their use for variable selection through synthetic and real-data experiments. Section 4 summarizes the methodological and theoretical implications of our work, along with potential extensions. Proofs of the main theorems are detailed in Appendix A. Auxiliary lemmas, corollaries and additional technical results are collected in the Supplementary Materials.

2 Main results

2.1 The degrees of freedom of Adaptive Lasso

Let $\mathbf{X}$, $\mathbf{y}$, $\boldsymbol{\beta}$ and γ as in the previous section, and $\mathbf{w} \in \mathbb{R}_+^p$ a vector of non-negative weights. Adaptive Lasso (Zou, 2006) estimator is defined as

$$\widehat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} \frac{1}{2}\|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2 + \gamma \sum_{j=1}^p w_j|\beta_j|. \tag{4}$$

The weights are chosen in a data-dependent way, often being a continuous positive function of the least squares estimates, $w_j = f(\widehat{\beta}_j^{\mathsf{LS}})$. Typical choices are $f(\widehat{\beta}_j^{\mathsf{LS}}) = 1/|\widehat{\beta}_j^{\mathsf{LS}}|^\alpha$ or $f(\widehat{\beta}_j^{\mathsf{LS}}) = \exp(-\alpha|\widehat{\beta}_j^{\mathsf{LS}}|)$, with $\alpha > 0$. Let $\mathcal{G} = \{1, \ldots, p\}$. The active set, i.e. the index set of nonzero estimates, sorted in increasing order, is denoted by

$$\mathcal{A} = \left\{ j \in \mathcal{G} : |\widehat{\beta}_j| \neq 0 \right\}.$$

The set $\mathcal{A}$ is clearly dependent on the data and the values γ but we omit this details for ease of notation. Calculation of the degrees of freedom involves the computation of the trace of $\partial\widehat{\mathbf{y}}_\gamma/\partial\mathbf{y}$. While for Lasso this result simplifies to the size of the active set (Zou et al., 2007), for its adaptive version the presence of data-dependent weights makes its calculation less straightforward. We are now ready to present the first contribution of our paper, which is an unbiased estimator of the degrees of freedom for Adaptive Lasso model in Equation (4) for general expression of the adaptive weights.

Theorem 1. *Let $\widehat{\boldsymbol{\beta}}$ the solution to the Adaptive Lasso problem in Equation (4) with weights $w_j = w_j(|\widehat{\beta}_j^{\mathsf{LS}}|)$ and $\gamma \in (\gamma_l, \gamma_{l+1})$. Denote with $\mathcal{A}$ the corresponding active set, and with $\mathbf{X}_\mathcal{A}$ the design matrix restricted to the active set. Define a mapping $\pi : \mathcal{A} \to \{1, 2, \ldots, |\mathcal{A}|\}$ such that for each $j \in \mathcal{A}$, $\pi(j) = i$ if $\mathcal{A}_i = j$. An unbiased estimate of the degrees of freedom is*

$$\widehat{df}_\gamma = |\mathcal{A}| - \gamma \sum_{j \in \mathcal{A}} \left.\frac{\partial w_j(z)}{\partial z}\right|_{z = \widehat{\beta}_j^{\mathsf{LS}}}, \tag{5}$$

for the orthonormal design and

$$\widehat{df}_\gamma = |\mathcal{A}| - \gamma \sum_{j \in \mathcal{A}} \operatorname{sgn}(\widehat{\beta}_j)\operatorname{sgn}(\widehat{\beta}_j^{\mathsf{LS}}) \left.\frac{\partial w_j(z)}{\partial z}\right|_{z = \widehat{\beta}_j^{\mathsf{LS}}} [(\mathbf{X}_\mathcal{A}^\top \mathbf{X}_\mathcal{A})^{-1}]_{\pi(j),\pi(j)}, \tag{6}$$

for non-orthonormal designs.

We now focus on the popular choice $w_j = 1/|\widehat{\beta}_j^{\mathsf{LS}}|$ for $j = 1, \ldots, G$ and specify the previous result for both the orthonormal and non-orthonormal cases. Analogous results for the less common case $w_j = \exp(-\alpha|\widehat{\beta}_j^{\mathsf{LS}}|)$ are presented in Corollary S.1 and S.2 of the Supplementary Materials.

Corollary 1. *Let $\mathbf{X}^\top\mathbf{X} = \mathbf{I}_p$ and $w_j = 1/|\widehat{\beta}_j^{\mathsf{LS}}|$. Under the settings of Theorem 1 an unbiased estimate of the degrees of freedom is*

$$\widehat{df}_\gamma = |\mathcal{A}| + \gamma \sum_{j \in \mathcal{A}} \frac{1}{(\widehat{\beta}_j^{\mathsf{LS}})^2}. \tag{7}$$

Corollary 2. *Let $\mathbf{X}^\top\mathbf{X} \neq \mathbf{I}_p$ and $w_j = 1/|\widehat{\beta}_j^{\mathsf{LS}}|$. Under the settings of Theorem 1 an unbiased estimate of the degrees of freedom is*

$$\widehat{df}_\gamma = |\mathcal{A}| + \gamma \sum_{j \in \mathcal{A}} \operatorname{sgn}(\widehat{\beta}_j) \frac{\operatorname{sgn}(\widehat{\beta}_j^{\mathsf{LS}})}{(\widehat{\beta}_j^{\mathsf{LS}})^2} [(\mathbf{X}_\mathcal{A}^\top \mathbf{X}_\mathcal{A})^{-1}]_{\pi(j),\pi(j)}. \tag{8}$$

Equations (7) and (8) reveal that the degrees of freedom extend beyond simply counting the active set size. Specifically, they include an additional term that depends on the weights' choice and on the regularization parameter γ. For non-orthonormal designs, the sign of the Adaptive Lasso estimate $\widehat{\boldsymbol{\beta}}$, the sign and magnitude of the least squares estimate $\widehat{\boldsymbol{\beta}}^{\mathsf{LS}}$ and the diagonal elements of the active set's precision matrix must also be incorporated. Notably, the degrees of

freedom expression exhibits a piecewise linear structure. This result stands in sharp contrast to the Lasso, where the estimated degrees of freedom form a piecewise constant function of γ. Consistently, $\widehat{df}_\gamma \geq |\mathcal{A}|$ demonstrating that the common practice of using only the active set size systematically underestimates the true degrees of freedom. The Lasso's piecewise constant degrees of freedom, however, can be recovered as a special case of the Adaptive Lasso by choosing fixed weights w_j. In this scenario, the gradient $\partial w_j(\mathbf{y})/\partial \mathbf{y}$ vanishes for all $j \in \mathcal{G}$, reducing $\widehat{df}_\gamma$ to a piecewise constant function, consistent with classical Lasso results. Furthermore, under certain conditions, this relationship displays strictly positive but successively diminishing slopes. This is formalized in the following corollary.

Corollary 3. *Let $w_j(|\widehat{\beta}_j^{\mathsf{LS}}|)$ be decreasing functions of $|\widehat{\beta}_j^{\mathsf{LS}}|$ for all $j \in \mathcal{G}$. Denote with $\mathcal{A}$ the corresponding active set. If $\mathrm{sgn}(\widehat{\beta}_j) \cdot \mathrm{sgn}(\widehat{\beta}_j^{\mathsf{LS}}) \geq 0$, for all $j \in \mathcal{G}$ then, for $\gamma \in (\gamma_l, \gamma_{l+1})$, $\widehat{df}_\gamma = |\mathcal{A}| + b_l\gamma$ with $b_l > 0$ for any $l = 1, \ldots, L-1$, leading to $\widehat{df}_\gamma > |\mathcal{A}|$. If the size of active set is a decreasing function of γ, then $b_l > b_{l+1}$ for any $l = 1, \ldots, L-1$.*

The conditions of Corollary 3 are typically satisfied in practice, as standard weights are usually monotonically decreasing functions of the absolute value of least squares estimates. The remaining two conditions, pertaining to the signs of the estimates and the size of the active set, are also frequently met in general settings and are guaranteed to hold for orthogonal designs. A counterintuitive property emerges from Corollary 3: within adjacent intervals defined by the transition points the estimated degrees of freedom $\widehat{df}_\gamma$ may be higher for $\gamma \in (\gamma_l, \gamma_{l+1})$ than for $\gamma \in (\gamma_{l-1}, \gamma_l)$ even if the active set size is actually decreased. This implies that a larger γ (and thus stronger regularization) does not always correspond to a simpler model, at least in terms of *effective complexity*, in line with the results of Kaufman and Rosset (2014) and Janson et al. (2015). This apparent inconsistency arises because, as already discussed, $\widehat{df}_\gamma$ depends not only on the number of active parameters but also on their adaptive weighting structure. When γ crosses a transition point γ_l, the adaptive weights—which themselves depend on $\mathbf{y}$—induce nonlinear interactions between the retained coefficients and the regularization path. These interactions can amplify the sensitivity of the fitted model to the data, effectively "consuming more information" despite a sparser active set.

2.2   The degrees of freedom of Group Lasso

Let $\mathbf{X}$, $\mathbf{y}$, $\boldsymbol{\beta}$ and γ as in the previous section. Let $G \leq p \in \mathbb{N}$, be the number of groups and $\mathbf{w} \in \mathbb{R}_+^G$ a vector of non-negative weights associated to each group. The Group Lasso (Yuan and Lin, 2006) estimator is defined as

$$\widehat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} \frac{1}{2}\|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2 + \gamma \sum_{g=1}^{G} w_g \|\boldsymbol{\beta}_g\|_2. \tag{9}$$

For this problem the group weights w_g are assumed to be independent from the response, a common choice being setting $w_g \propto n_g$ where n_g is the size of the corresponding group. If the weights are determined in an *adaptive* way, then the model is known as Adaptive Group Lasso (Wang and Leng, 2008) for which we provide results in the following Section 2.3. For the Group Lasso, let $\mathcal{G}_p = \{1, \ldots, p\}$ be the index set of all variables and $\mathcal{G}_G = \{1, \ldots, G\}$ the index set of all groups. Then, define the index set of active variables and the index set of active groups as

$$\mathcal{A}_p = \left\{ j \in \mathcal{G}_p : |\widehat{\beta}_j| \neq 0 \right\}, \qquad \mathcal{A}_G = \left\{ g \in \mathcal{G}_G : \|\widehat{\boldsymbol{\beta}}_g\|_2 \neq 0 \right\}.$$

Again, we omit the hat from $\mathcal{A}_p$ and $\mathcal{A}_G$, as well as their dependence from γ. We are now ready to state the main result about the computation of degrees of freedom of Group Lasso under the orthonormal design.

Theorem 2. *Let* $\mathbf{X}^\top\mathbf{X} = \mathbf{I}_p$, $\widehat{\boldsymbol{\beta}}$ *be the solution to the Group Lasso problem in Equation* (9) *with groups cardinality equal to* $n_1, \ldots, n_G$, *and* $\gamma \in (\gamma_l, \gamma_{l+1})$. *Denote with* $\mathcal{A}_G$ *the corresponding active group set. An unbiased estimate of the degrees of freedom is*

$$\widehat{df}_\gamma = \mathrm{trace}\big[(\mathbf{I}_n + \gamma\mathbf{B})^{-1}\mathbf{A}\big], \tag{10}$$

where $\mathbf{A} = \mathbf{X}_{\mathcal{A}_G}\mathbf{X}_{\mathcal{A}_G}^\top$, $\mathbf{B} = \mathbf{X}_{\mathcal{A}_G}\mathbf{\Pi}_{\mathcal{A}_G}\mathbf{X}_{\mathcal{A}_G}^\top$, *and*

$$\mathbf{\Pi}_{\mathcal{A}_G} = \mathrm{blockdiag}\bigg(w_g\bigg[\frac{\mathbf{I}_{n_g}}{\|\widehat{\boldsymbol{\beta}}_g\|_2} - \frac{\widehat{\boldsymbol{\beta}}_g\widehat{\boldsymbol{\beta}}_g^\top}{\|\widehat{\boldsymbol{\beta}}_g\|_2^3}\bigg]\bigg). \tag{11}$$

We now consider the more general case where the design matrix is not orthonormal.

Theorem 3. *Let* $\mathbf{X}^\top\mathbf{X} \neq \mathbf{I}_p$, $\widehat{\boldsymbol{\beta}}$ *the solution to the Group Lasso problem in Equation* (9) *with groups cardinality equal to* $n_1, \ldots, n_G$ *and* $\gamma \in (\gamma_l, \gamma_{l+1})$. *Denote with* $\mathcal{A}_G$ *the corresponding active group set. An unbiased estimate of the degrees of freedom is*

$$\widehat{df}_\gamma = \mathrm{trace}\big[(\mathbf{I}_n + \gamma\mathbf{B})^{-1}\mathbf{A}\big], \tag{12}$$

where $\mathbf{A} = \mathbf{X}_{\mathcal{A}_G}(\mathbf{X}_{\mathcal{A}_G}^\top\mathbf{X}_{\mathcal{A}_G})^{-1}\mathbf{X}_{\mathcal{A}_G}^\top$, $\mathbf{B} = \mathbf{X}_{\mathcal{A}_G}(\mathbf{X}_{\mathcal{A}_G}^\top\mathbf{X}_{\mathcal{A}_G})^{-1}\mathbf{\Pi}_{\mathcal{A}_G}(\mathbf{X}_{\mathcal{A}_G}^\top\mathbf{X}_{\mathcal{A}_G})^{-1}\mathbf{X}_{\mathcal{A}_G}^\top$, *and*

$$\mathbf{\Pi}_{\mathcal{A}_G} = \mathrm{blockdiag}\bigg(w_g\bigg[\frac{\mathbf{I}_{n_g}}{\|\widehat{\boldsymbol{\beta}}_g\|_2} - \frac{\widehat{\boldsymbol{\beta}}_g\widehat{\boldsymbol{\beta}}_g^\top}{\|\widehat{\boldsymbol{\beta}}_g\|_2^3}\bigg]\bigg).$$

The results in Equations (10) and (12) are apparently different from those of the Lasso and Adaptive Lasso. Furthermore, Equation (10) looks different from that reported in the original Group Lasso paper by Yuan and Lin (2006) and from a related expression reported by Vaiter et al. (2017). The relations between these expressions are further discussed in Corollary S.3 in the Supplementary Materials. From Equations (10) and (12), it becomes evident that an unbiased estimate of the degrees of freedom for Group Lasso is again not merely the trace of the projection matrix—which would equate to the number of active variables—but rather the trace of a slightly different matrix. This matrix additionally depends on the design matrix and the vector of estimated coefficients. Consistently, using the size of the active set as an estimator of the degrees of freedom is generally not valid for Group Lasso. The following corollary provides bounds for the degrees of freedom obtained in Theorems 2 and 3.

Corollary 4. *The estimated degrees of freedom of Group Lasso given by Theorem 2 and 3 are a continuous function of* γ, *for* $\gamma \in (\gamma_l, \gamma_{l+1})$ *and*

$$|\mathcal{A}_G| \;\leq\; \widehat{df}_\gamma \;\leq\; |\mathcal{A}_p|,$$

where we have $|\mathcal{A}_G| = \widehat{df}_\gamma = |\mathcal{A}_p| = 0$ *if there are no active groups, and* $\widehat{df}_\gamma = |\mathcal{A}_p| = p$ *in the limiting case* $\gamma = 0$ *of no penalization.*

Differently from Lasso, in Group Lasso the Stein's estimator of degrees of freedom lead to a non-constant piecewise continuous function. This means that by replacing the ℓ_1 norm with the ℓ_2 norm we lose the perfect balance, typical of the Lasso, between using the response for variable selection and applying shrinkage. Specifically, the estimated degrees of freedom of Group Lasso are always lower than $|\mathcal{A}_p|$, being equal to such value only in limiting cases. Thus the use of the ℓ_2 norm results in a more parsimonious usage of the information available in data. As expected, we recover the Lasso's expression if we set the number of elements in each group to one, as formally discussed in Corollary S.4 in the Supplementary Materials. A natural question is whether the estimated degrees of freedom of the Group Lasso decrease as γ increases. The answer is formalized in the next two theorems.

Theorem 4. *If the matrix $\mathbf{\Pi}_{\mathcal{A}_G} + \gamma \mathrm{d}\mathbf{\Pi}_{\mathcal{A}_G}/\mathrm{d}\gamma$ is positive definite, then the estimated degrees of freedom of Group Lasso given by Theorem 2 and 3 are non-increasing function of γ, for $\gamma \in (\gamma_l, \gamma_{l+1})$.*

Theorem 5. *If $\mathbf{X}^\top \mathbf{X} = \mathbf{I}_p$ or $\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}$ is an eigenvector of the matrix $(\mathbf{X}_{\mathcal{A}_G}^\top \mathbf{X}_{\mathcal{A}_G} + \gamma \mathbf{\Pi}_{\mathcal{A}_G})^{-1} \mathbf{W}_{\mathcal{A}_G}$, the matrix $\mathbf{\Pi}_{\mathcal{A}_G} + \gamma \mathrm{d}\mathbf{\Pi}_{\mathcal{A}_G}/\mathrm{d}\gamma$ is positive semidefinite. Otherwise, it is indefinite.*

Corollary 5. *For a general design matrix, monotonicity of the estimated degrees of freedom cannot be established by positive semidefiniteness of the matrix $\mathbf{\Pi}_{\mathcal{A}_G} + \gamma \mathrm{d}\mathbf{\Pi}_{\mathcal{A}_G}/\mathrm{d}\gamma$, in general. Nevertheless, by leveraging Lemma 5 in the Supplementary Materials, a sufficient condition is $\mathrm{trace}(\mathbf{A}\mathbf{B}) > 0$, where $\mathbf{A} = \mathbf{\Pi}_{\mathcal{A}_G} + \gamma \mathrm{d}\mathbf{\Pi}_{\mathcal{A}_G}/\mathrm{d}\gamma$ $\mathbf{B} = \mathbf{M}_{\mathcal{A}_G}^\top (\mathbf{I}_n + \gamma \mathbf{B}_\gamma)^{-1} \mathbf{A} (\mathbf{I}_n + \gamma \mathbf{B}_\gamma)^{-1} \mathbf{M}_{\mathcal{A}_G}$, $\mathbf{M}_{\mathcal{A}_G} = \mathbf{X}_{\mathcal{A}_G}(\mathbf{X}_{\mathcal{A}_G}^\top \mathbf{X}_{\mathcal{A}_G})^{-1}$.*

The contribution of Theorems 4 and 5 is the characterization of the gradient of the estimated degrees of freedom of the Group Lasso in terms of the spectral decomposition of the matrix $\mathbf{\Pi}_{\mathcal{A}_G} + \gamma \mathrm{d}\mathbf{\Pi}_{\mathcal{A}_G}/\mathrm{d}\gamma$. This spectral perspective provides a fine-grained understanding of the underlying geometric and algebraic mechanisms that govern the behavior of the estimator as the regularization parameter γ varies. Consistently, the results presented in such theorems, and the associated corollaries in the Supplementary Materials, constitute a substantial advancement in understanding the estimated degrees of freedom of the Group Lasso. In particular, these results go significantly beyond the existing literature by providing an explicit and general expression for the derivative of the estimated degrees of freedom with respect to γ, valid under general non-orthogonal design conditions. Previous studies typically restrict attention to the orthonormal design case, under which significant simplifications arise. Specifically, only in the orthonormal setting the matrix $\mathbf{\Pi}_{\mathcal{A}_G} + \gamma \mathrm{d}\mathbf{\Pi}_{\mathcal{A}_G}/\mathrm{d}\gamma$ is positive semidefinite, as stated in Theorem 5. In this case, negative eigenvalues vanish, while the other eigenvalues reduce to simple closed-form expressions. Moreover, in this settings the matrices $\mathbf{\Pi}_g$, as well as vectors $\widehat{\boldsymbol{\beta}}_g$ and their norms, scale linearly with γ for each active group $g \in \mathcal{A}_G$, as established in Corollary S.5 in the Supplementary Materials, indicating a smooth shrinkage along each of the directions $\widehat{\boldsymbol{\beta}}_g$. Notably, this behavior no longer holds in the general non-orthogonal design case. In fact, in the general non-orthogonal case, the analysis rigorously reveals that the matrix $\mathbf{\Pi}_{\mathcal{A}_G} + \gamma \mathrm{d}\mathbf{\Pi}_{\mathcal{A}_G}/\mathrm{d}\gamma$ becomes indefinite, and monotonicity of the estimated degrees of freedom should be established by other sufficient conditions, as outlined for instance in Corollary 5.

2.3 The degrees of freedom of Adaptive Group Lasso

Let $\mathbf{X}$, $\mathbf{y}$, $\boldsymbol{\beta}$, γ, and G as in the previous sections. Let $\mathbf{w}(\mathbf{y}) \in \mathbb{R}_+^G$ a vector of non-negative data-dependent weights associated to each group. The Adaptive Group Lasso estimator is defined as

$$\widehat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} \frac{1}{2}\|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2 + \gamma \sum_{g=1}^{G} w_g(\mathbf{y})\|\boldsymbol{\beta}_g\|_2. \tag{13}$$

As in previous section, let $\mathcal{A}_p$ and $\mathcal{A}_G$ bet the index sets of active groups and active variables, respectively. We are now ready to present the unbiased estimator for the degrees of freedom in Adaptive Group Lasso model in Equation (13) under general expression for the adaptive weights.

Theorem 6. *Let $\widehat{\boldsymbol{\beta}}$ be the solution to the Adaptive Group Lasso problem in Equation (13) with groups cardinality equal to $n_1, \ldots, n_G$, weights defined as $w_g = w_g(\|\widehat{\boldsymbol{\beta}}^{\mathsf{LS}}\|_2)$ and $\gamma \in (\gamma_l, \gamma_{l+1})$. Denote with $\mathcal{A}_G$ the corresponding active group set, and with $\mathbf{X}_{\mathcal{A}_G}$ the design matrix restricted to the active group set. An unbiased estimate of the degrees of freedom is*

$$\widehat{df}_\gamma = \mathrm{trace}\big[(\mathbf{I}_n + \gamma \mathbf{B})^{-1}(\mathbf{A} - \gamma \mathbf{C})\big], \tag{14}$$

where $\mathbf{A} = \mathbf{X}_{\mathcal{A}_G}\mathbf{X}_{\mathcal{A}_G}^\top$, $\mathbf{B} = \mathbf{X}_{\mathcal{A}_G}\mathbf{\Pi}_{\mathcal{A}_G}\mathbf{X}_{\mathcal{A}_G}^\top$, $\mathbf{C} = \mathbf{X}_{\mathcal{A}_G}\mathbf{\Phi}_{\mathcal{A}_G}\mathbf{X}_{\mathcal{A}_G}^\top$ *for the orthonormal design,*
$\mathbf{A} = \mathbf{X}_{\mathcal{A}_G}(\mathbf{X}_{\mathcal{A}_G}^\top\mathbf{X}_{\mathcal{A}_G})^{-1}\mathbf{X}_{\mathcal{A}_G}^\top$, $\mathbf{B} = \mathbf{X}_{\mathcal{A}_G}(\mathbf{X}_{\mathcal{A}_G}^\top\mathbf{X}_{\mathcal{A}_G})^{-1}\mathbf{\Pi}_{\mathcal{A}_G}(\mathbf{X}_{\mathcal{A}_G}^\top\mathbf{X}_{\mathcal{A}_G})^{-1}\mathbf{X}_{\mathcal{A}_G}^\top$,
$\mathbf{C} = \mathbf{X}_{\mathcal{A}_G}(\mathbf{X}_{\mathcal{A}_G}^\top\mathbf{X}_{\mathcal{A}_G})^{-1}\mathbf{\Phi}_{\mathcal{A}_G}(\mathbf{X}_{\mathcal{A}_G}^\top\mathbf{X}_{\mathcal{A}_G})^{-1}\mathbf{X}_{\mathcal{A}_G}^\top$ *for non-orthonormal designs, and*

$$\mathbf{\Pi}_{\mathcal{A}_G} = \mathrm{blockdiag}\left(w_g\left[\frac{\mathbf{I}_{n_g}}{\|\widehat{\boldsymbol{\beta}}_g\|_2} - \frac{\widehat{\boldsymbol{\beta}}_g\widehat{\boldsymbol{\beta}}_g^\top}{\|\widehat{\boldsymbol{\beta}}_g\|_2^3}\right]\right), \quad \mathbf{\Phi}_{\mathcal{A}_G} = \mathrm{blockdiag}\left(\frac{\widehat{\boldsymbol{\beta}}_g}{\|\widehat{\boldsymbol{\beta}}_g\|_2}\frac{\partial w_g(\|\widehat{\boldsymbol{\beta}}^{\mathsf{LS}}\|_2)}{\partial\|\widehat{\boldsymbol{\beta}}^{\mathsf{LS}}\|_2}\frac{(\widehat{\boldsymbol{\beta}}^{\mathsf{LS}})^\top}{\|\widehat{\boldsymbol{\beta}}^{\mathsf{LS}}\|_2}\right).$$

Notably, these expressions incorporate two competing effects: an inflation effect caused by the use of adaptive weights, consistently with Section 2.1, and a contraction effect induced by the ℓ_2 norm, consistently with Section 2.2. The relative strength of the two parts cannot be generally determined, and wether the trace of this quantity is greater or lower than $|\mathcal{A}_p|$ is not known. We now specify the expression for the degrees of freedom of Group Lasso with adaptive weights for both orthonormal and non-orthonormal designs, under the typical assumption for the weights $w_g = 1/\|\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}}\|_2$.

Corollary 6. *Let* $\mathbf{X}^\top\mathbf{X} = \mathbf{I}_p$ *and* $w_g = 1/\|\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}}\|_2$. *Under the settings of Theorem 6 an unbiased estimate of the degrees of freedom is*

$$\widehat{df}_\gamma = \mathrm{trace}\big[(\mathbf{I}_n + \gamma\mathbf{B})^{-1}(\mathbf{A} + \gamma\mathbf{C})\big], \tag{15}$$

where $\mathbf{A} = \mathbf{X}_{\mathcal{A}_G}\mathbf{X}_{\mathcal{A}_G}^\top$, $\mathbf{B} = \mathbf{X}_{\mathcal{A}_G}\mathbf{\Pi}_{\mathcal{A}_G}\mathbf{X}_{\mathcal{A}_G}^\top$, $\mathbf{C} = \mathbf{X}_{\mathcal{A}_G}\mathbf{\Phi}_{\mathcal{A}_G}\mathbf{X}_{\mathcal{A}_G}^\top$, *and*

$$\mathbf{\Pi}_{\mathcal{A}_G} = \mathrm{blockdiag}\left(w_g\left[\frac{\mathbf{I}_{n_g}}{\|\widehat{\boldsymbol{\beta}}_g\|_2} - \frac{\widehat{\boldsymbol{\beta}}_g\widehat{\boldsymbol{\beta}}_g^\top}{\|\widehat{\boldsymbol{\beta}}_g\|_2^3}\right]\right), \qquad \mathbf{\Phi}_{\mathcal{A}_G} = \mathrm{blockdiag}\left(\frac{\widehat{\boldsymbol{\beta}}_g}{\|\widehat{\boldsymbol{\beta}}_g\|_2}\frac{(\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}})^\top}{\|\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}}\|_2^3}\right).$$

Corollary 7. *Let* $\mathbf{X}^\top\mathbf{X} \neq \mathbf{I}_p$ *and* $w_g = 1/\|\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}}\|_2$. *Under the settings of Theorem 6 an unbiased estimate of the degrees of freedom is*

$$\widehat{df}_\gamma = \mathrm{trace}\big[(\mathbf{I}_n + \gamma\mathbf{B})^{-1}(\mathbf{A} + \gamma\mathbf{C})\big], \tag{16}$$

where $\mathbf{A} = \mathbf{X}_{\mathcal{A}_G}(\mathbf{X}_{\mathcal{A}_G}^\top\mathbf{X}_{\mathcal{A}_G})^{-1}\mathbf{X}_{\mathcal{A}_G}^\top$, $\mathbf{B} = \mathbf{X}_{\mathcal{A}_G}(\mathbf{X}_{\mathcal{A}_G}^\top\mathbf{X}_{\mathcal{A}_G})^{-1}\mathbf{\Pi}_{\mathcal{A}_G}(\mathbf{X}_{\mathcal{A}_G}^\top\mathbf{X}_{\mathcal{A}_G})^{-1}\mathbf{X}_{\mathcal{A}_G}^\top$,
$\mathbf{C} = \mathbf{X}_{\mathcal{A}_G}(\mathbf{X}_{\mathcal{A}_G}^\top\mathbf{X}_{\mathcal{A}_G})^{-1}\mathbf{\Phi}_{\mathcal{A}_G}(\mathbf{X}_{\mathcal{A}_G}^\top\mathbf{X}_{\mathcal{A}_G})^{-1}\mathbf{X}_{\mathcal{A}_G}^\top$, *and*

$$\mathbf{\Pi}_{\mathcal{A}_G} = \mathrm{blockdiag}\left(w_g\left[\frac{\mathbf{I}_{n_g}}{\|\widehat{\boldsymbol{\beta}}_g\|_2} - \frac{\widehat{\boldsymbol{\beta}}_g\widehat{\boldsymbol{\beta}}_g^\top}{\|\widehat{\boldsymbol{\beta}}_g\|_2^3}\right]\right), \qquad \mathbf{\Phi}_{\mathcal{A}_G} = \mathrm{blockdiag}\left(\frac{\widehat{\boldsymbol{\beta}}_g}{\|\widehat{\boldsymbol{\beta}}_g\|_2}\frac{(\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}})^\top}{\|\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}}\|_2^3}\right).$$

Similarly to Corollary 3 we can compare the degrees of freedom in Equation (14) with those of the Group Lasso. Specifically, we show that under certain conditions the Adaptive Group Lasso degrees of freedom estimates are no lower than those of the Group Lasso. This is formalized in the following Corollary.

Corollary 8. *Let* $w_g(\|\widehat{\boldsymbol{\beta}}_g\|_2)$ *be decreasing functions of* $\|\widehat{\boldsymbol{\beta}}_g\|_2$ *for all* $g \in \mathcal{G}_G$. *If* $\widehat{\boldsymbol{\beta}}_g^\top\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}} \geq 0$, *for all* $g \in \mathcal{G}_G$ *then, for* $\gamma \in (\gamma_l, \gamma_{l+1})$, $\widehat{df}_\gamma$ *for Adaptive Group Lasso, as defined in Equation (14), are bounded below by* $\widehat{df}_\gamma$ *for Group Lasso, as defined in Equation (10) and (12), for any* $l = 1, \ldots, L-1$.

In the orthonormal design setting, an alternative expression for the estimated degrees of freedom appearing in Equation (15) in the spirit of Yuan and Lin (2006) can be derived, and it is presented in Corollary S.6 in the Supplementary Materials. In the same document, Corollary S.7 shows that Lasso and Group Lasso are special cases of Adaptive Group Lasso, and their estimated degrees of freedom can be recovered from Theorem 6.
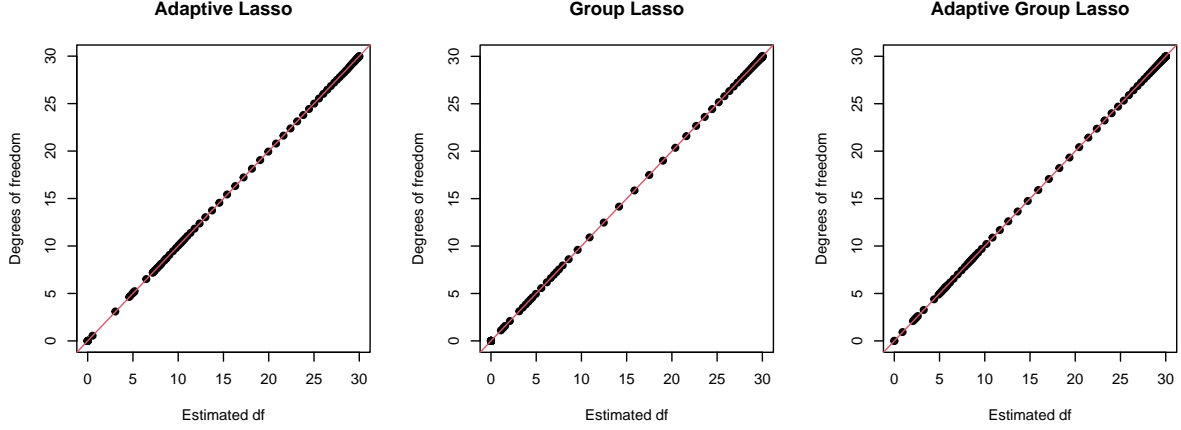
Figure 1: Estimated degrees of freedom using the appropriate theorem (x axis) versus degrees of freedom computed with the general covariance formula (1) *for Adaptive Lasso, Group Lasso and Adaptive Group Lasso.*

3 Empirical Assessment

In this section, we conduct two numerical experiments to validate and contextualize our theoretical findings. First, we generate synthetic data to empirically demonstrate the consistency of our theoretical results. Second, we analyze a real-world dataset to evaluate the utility of the estimated degrees of freedom in model selection. Notably, the use of our results achieves performance comparable to computationally intensive cross-validation while diverging significantly from the naive practice of equating the degrees of freedom to the size of the active set.

3.1 Synthetic data

We let $n = 100$ and $p = 30$ and generate a $n \times p$ data matrix $\mathbf{X} = (\mathbf{X}_1, \ldots, \mathbf{X}_p)$ where $\mathbf{X}_j \sim \mathrm{N}(0, \mathbf{I}_n)$ for $j = 1, \ldots, p$. We fix $\boldsymbol{\beta} = (5, -5, 5, 3, -3, 3, 1, -1, 1, 0, \ldots, 0)$ thus having the last 21 coefficients equal to zero, and consequently let $\mathbf{y}^\star = \mathbf{X}\boldsymbol{\beta}$. For $B = 10{,}000$ replications we perturb $\mathbf{y}^\star$ with independent noise generated from a Gaussian distribution with zero mean and variance equal to a value leading to a signal-to-noise ratio equal to 4, obtaining $\mathbf{y}_b = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}_b$. Estimation of $\boldsymbol{\beta}$ is obtained with the estimators presented in Equations (4), (9), and (13). For the Group Lasso and its adaptive version, we grouped three consecutive coefficients leading to $n_g = 3$ for $g = 1, \ldots, G$ and $G = 10$. For the Adaptive Lasso, weights are equal to the reciprocal of the absolute values of least squares estimates of the parameters. For the Adaptive Group lasso the weight of each group equals the reciprocal of the ℓ_2 norm of corresponding least squares estimates. For each method, an appropriate range for the regularization parameter is considered, and the entire path of solutions of the corresponding optimization problem is computed. For each replicate $b = 1, \ldots, B$, we compute the estimated degrees of freedom using results of Theorems 1, 2, and 6, respectively. The unbiasedness of these estimators is verified by comparing their empirical average with the theoretical degrees of freedom computed via the covariance formula in Equation (1). Figure 1 demonstrates strong agreement across all methods. Note that while Equation (1) serves as a benchmark, it cannot be applied in practice as it requires knowledge of the true parameter values. Additionally, for each replicate, we determine the optimal regularization parameter γ with respect to the BIC by minimizing the expression in Equation (3). Here, the degrees of freedom are computed using the method

corresponding to each regularization technique, and σ^2 replaced by its estimate obtained from ordinary linear regression. The distribution of the number of retained coefficients across the B replicates, corresponding to each optimal γ, is presented in Table 1. The results indicate that Adaptive Lasso and Adaptive Group Lasso select 9 variables in the majority of cases, whereas Group Lasso frequently retains more than 9. This discrepancy arises because Group Lasso, lacking an adaptive mechanism, often fails to exclude noise-related coefficients.

Table 1: Empirical distribution of variables entering the model over 10000 repetitions (the true value is 9) for Adaptive Lasso, Group Lasso, and Adaptive Group Lasso.

	≤ 7	8	**9**	10	11	12	≥ 13
Adaptive Lasso	341	1154	4385	2217	1042	461	400
Group Lasso	0	0	3786	0	0	3358	2856
Adaptive Group Lasso	9	0	9449	0	0	504	38

3.2   Diabetes data

To illustrate the utility of our findings we analyze the Diabetes dataset (Efron et al., 2004; Zou et al., 2007). This dataset is available in two versions: a *small* version with $p = 10$ covariates, and a *large* version with $p = 64$ covariates. The number of observations is $n = 442$. The covariates are individual characteristics and biomarkers while the response variable is a quantitative measure of disease progression. We use this dataset to illustrate our results with two separate analyses. First, we use the original $p = 10$ covariates of the *small* version and fit a linear model with Lasso and Adaptive Lasso penalties discussing model selection via BIC. In a second analysis we discretize the continuous covariates into ordinal categorical variables for "high", "medium-high", "medium-low", and "low" levels of each biomarkers and encode these categorical variable into three dummy variables for each biomarker. After defining groups of dummy variable associated to the same categorical variable, we fit linear regression models with Group Lasso and Adaptive Group Lasso penalties. We start by discussing the results for the Lasso and Adaptive Lasso. The upper panels of Figure 2 report the estimated degrees of freedom as a function of $\log(\gamma)$. For comparison, we include the size of the active set (shown as a dashed line) to highlight discrepancies arising from the common but erroneous practice of equating this quantity with the estimated degrees of freedom across all penalization methods. It can be seen that for the Adaptive lasso, the correct estimated degrees of freedom (solid curve) are strictly lower-bounded by the active set size. This reveals that using the active set size as a proxy for degrees of freedom systematically underestimates the true complexity of the model, leading to an incomplete characterization of the information utilized in parameter estimation. Notably, the upper right panel also demonstrates the behavior described by Corollary 3. Additionally, it can be noticed that, in some interval (γ_l, γ_{l+1}) the value of the estimated degrees of freedom in a left neighborhood of γ_{l+1} is actually higher than that for a left neighborhood of γ_l as also discussed as a comment of Corollary 3. The lower panels of Figure 2, instead, report complete solution paths for different values of γ. Solid vertical lines denote the γ values that minimize BIC according to Equation (3) when using the correct estimated degrees of freedom for each criterion. For comparison, dash-dotted vertical lines mark the optimal γ selected via leave-one-out cross-validation while, for the Adaptive Lasso, a dashed vertical line denotes the γ value that minimizes BIC using the size of the active set in place of the correct estimated degrees of freedom. A key difference emerges in this case, as the selected γ is larger. This reaffirms that misrepresenting
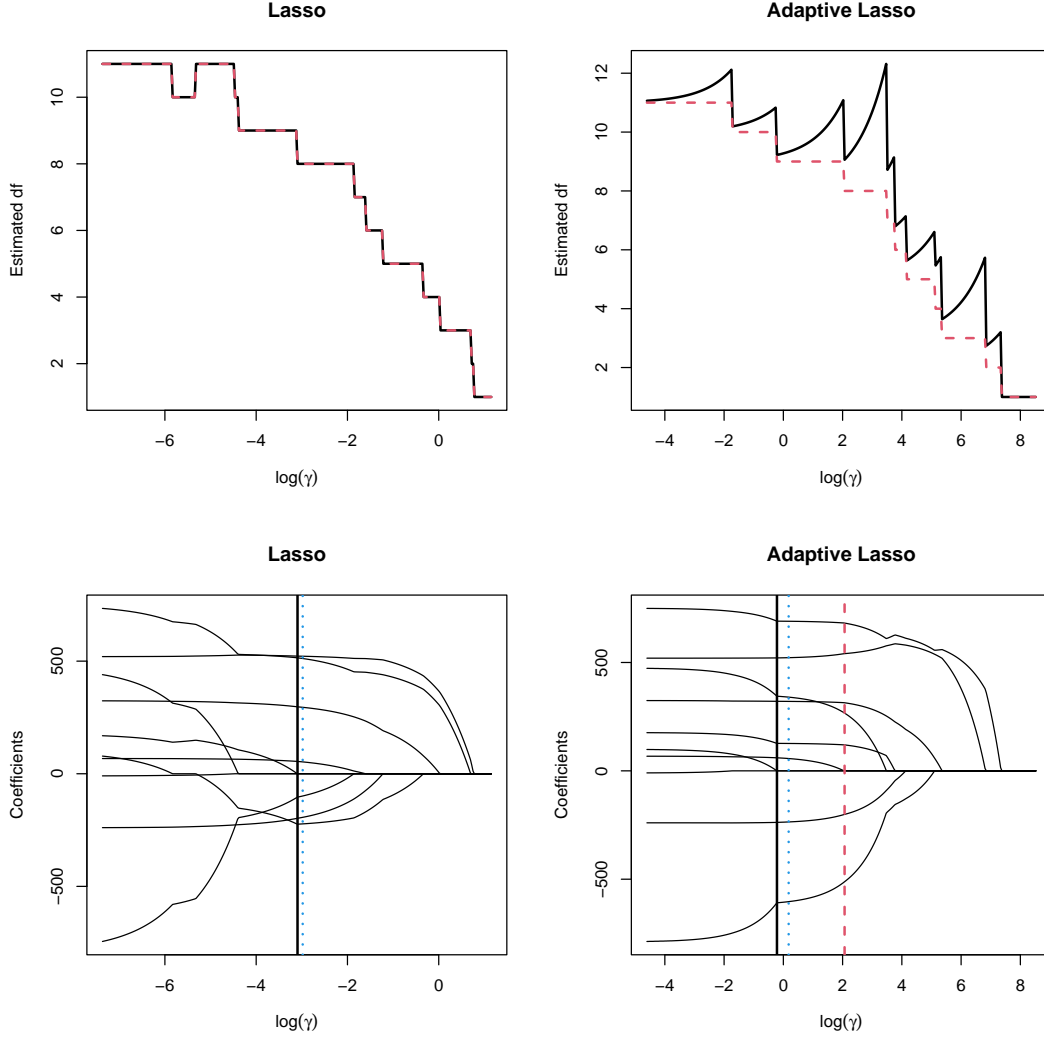
Figure 2: Results of the Lasso (left) and Adaptive Lasso (right) estimation for the Diabetes (small) data. Estimated degrees of freedom (upper panels, continuous lines) along with the size of the active set (dashed lines). Complete solution path (lower panels) with vertical lines denoting the best γ according to correct BIC (continuous line), cross validation (dotted line), BIC with active set size as estimator of the degrees of freedom (dashed).

degrees of freedom via the active set size here introduces bias, likely favoring over-regularized models. We continue our illustration discussing the results for the Group Lasso and Adaptive Group Lasso. The upper panels of Figure 3, similarly to Figure 2, report the estimated degrees of freedom as a function of $\log(\gamma)$. Also here the dashed lines in the up panels represent the active set. A gray dashed lines has been also added for the left up panel representing the size of the active groups. For the Group Lasso, the correct estimated degrees of freedom (solid curve) are strictly upper-bounded by the active set size. This, contrarily to the Adaptive Lasso, reveals that using the active set size as a proxy for degrees of freedom systematically overestimate the true complexity of the model. Moreover, as prescribed by Corollary 4, estimated degrees of freedom of Group Lasso are greater than the number of active groups, presented in Figure 3 as a dotted gray line. As discussed after the statement of Theorem 7, the Adaptive Group Lasso incorporates two competing effects: an inflation effect caused by the use of adaptive weights

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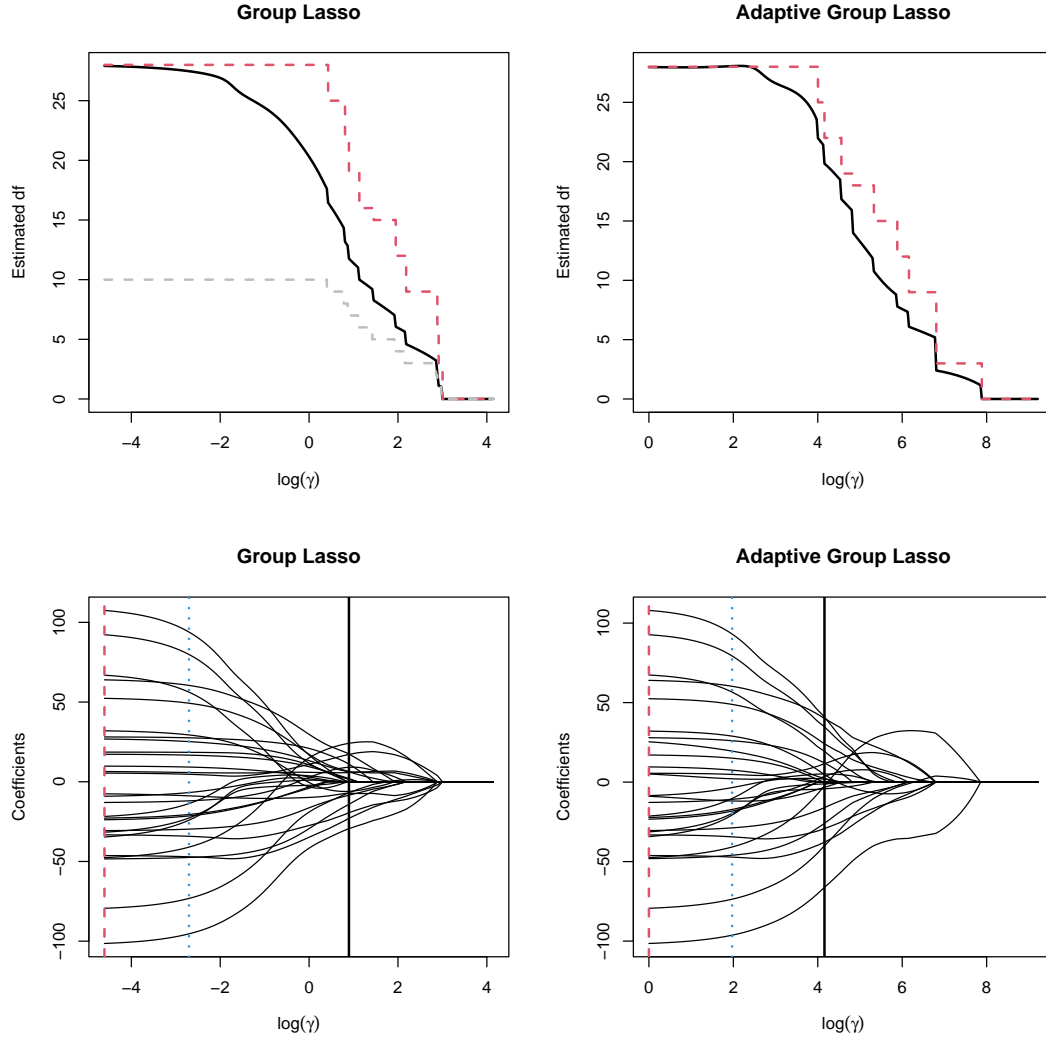
Figure 3: Results of the Group Lasso (left) and Adaptive Group Lasso (right) estimation for the Diabetes data with the covariates discretized and encoded as dummy variables. Estimated degrees of freedom (upper panels, continuous lines) along with the size of the active set (dashed lines). For the Group Lasso also the size of the active groups is reported (dashed gray lines). Complete solution path (lower panels) with vertical lines denoting the best γ according to correct BIC (continuous line), cross validation (dotted line), BIC with active set size as estimator of the degrees of freedom (dashed).

and a contraction effect induced by the ℓ_2 norm. In this specific case, the result is still upper bounded by the active set even though as can be noticed by the upper right panel of Figure 3. It should be noted, however, that in other cases, the two effects almost compensate leading a to an estimation for the degrees of freedom that is not so far from the size of the active set. The lower panels of Figure 3 instead, tell a similar story to those of Figure 2 with the γ chosen minimizing the correct BIC being closer to the leave-one-out cross validation choice than the one exploiting the BIC using the size of the active set in place of the correct degrees of freedom.

4   Conclusions

We introduced a general framework for computing unbiased estimates of the degrees of freedom in penalized regression models, extending the foundational work of Zou et al. (2007). Our theoretical results underline that the common practice of using the size of active set as an estimate of the degrees of freedom is biased in many respect. This practice can severely distort inference since the size of active set and the true degrees of freedom are usually different, as highlighted by Janson et al. (2015). For the Adaptive Lasso, for example, we demonstrated that the correct estimate includes, in addition to the active set size, an adjustment term whose sign depends on the weights' selection. Under default weighting schemes, this term is positive, leading to an inflation of the degrees of freedom relative to the active set size. In contrast, the Group Lasso exhibits a deflation effect due to its reliance on the ℓ_2 norm, reducing the degrees of freedom compared to the active set size. The Adaptive Group Lasso presents a more complex interplay: both inflation (from adaptive weights) and contraction (from ℓ_2 shrinkage) coexist, making general characterization difficult. In addition to the analytical expressions for the degrees of freedom, we provide deep understanding of their local behavior as functions of γ. Specifically, we show that for the Adaptive Lasso (under certain conditions), these exhibit strictly positive but monotonic decreasing slopes within adjacent change points. For the Group Lasso, we show that the associated degrees of freedom are bounded between the active groups and active coefficients, and their local monotonicity is intimately related to the notion of orthogonality. These findings advance the understanding of model complexity in penalized regression, with implications for model selection, risk estimation, and theoretical analysis of high-dimensional methods.

A   Proofs

Proof of Theorem 1. Let $\mathbf{W} = \mathrm{diag}(w_1, \ldots, w_p) \in \mathbb{S}^p_{++}$. The first order conditions for the problem in Equation (4) are represented by

$$-\mathbf{X}_{\mathcal{A}}^\top(\mathbf{y} - \mathbf{X}_{\mathcal{A}}\widehat{\boldsymbol{\beta}}_{\mathcal{A}}) + \gamma\mathbf{W}_{\mathcal{A}}\mathrm{sgn}(\widehat{\boldsymbol{\beta}}_{\mathcal{A}}) = \mathbf{0}, \tag{17}$$

where $\mathbf{X}_{\mathcal{A}}$, $\widehat{\boldsymbol{\beta}}_{\mathcal{A}}$, $\mathbf{W}_{\mathcal{A}}$ and $\mathrm{sgn}(\widehat{\boldsymbol{\beta}}_{\mathcal{A}})$ are restricted to the active set $\mathcal{A}$. It is important to note that Equation (17) is only valid for $\gamma \in (\gamma_l, \gamma_{l+1})$, where γ_l and γ_{l+1} are two consecutive *transition points* and for any $l = 1, \ldots, L - 1$. By manipulating Equation (17) we can derive an implicit equation for $\widehat{\boldsymbol{\beta}}_{\mathcal{A}}$,

$$\widehat{\boldsymbol{\beta}}_{\mathcal{A}} = (\mathbf{X}_{\mathcal{A}}^\top\mathbf{X}_{\mathcal{A}})^{-1}(\mathbf{X}_{\mathcal{A}}^\top\mathbf{y} - \gamma\mathbf{W}_{\mathcal{A}}\mathrm{sgn}(\widehat{\boldsymbol{\beta}}_{\mathcal{A}})),$$

and denoting

$$\mathbf{H}_{\gamma}(\mathbf{y}) = \mathbf{X}_{\mathcal{A}}(\mathbf{X}_{\mathcal{A}}^\top\mathbf{X}_{\mathcal{A}})^{-1}\mathbf{X}_{\mathcal{A}}^\top$$
$$\eta_{\gamma}(\mathbf{y}) = \mathbf{X}_{\mathcal{A}}(\mathbf{X}_{\mathcal{A}}^\top\mathbf{X}_{\mathcal{A}})^{-1}\mathbf{W}_{\mathcal{A}}\mathrm{sgn}(\widehat{\boldsymbol{\beta}}_{\mathcal{A}}),$$

we can also derive the equation linking $\widehat{\mathbf{y}}_{\gamma}$ and $\mathbf{y}$, i.e.

$$\widehat{\mathbf{y}}_{\gamma} = \mathbf{X}\widehat{\boldsymbol{\beta}} = \mathbf{H}_{\gamma}(\mathbf{y})\mathbf{y} - \gamma\eta_{\gamma}(\mathbf{y}).$$

In order to apply Equation (2), we need $\partial\widehat{\mathbf{y}}_{\gamma}/\partial\mathbf{y}$. Consider the increments $\mathbf{y} + \Delta\mathbf{y}$, then

$$\widehat{\mathbf{y}}_{\gamma}(\mathbf{y} + \Delta\mathbf{y}) = \mathbf{X}\widehat{\boldsymbol{\beta}}(\mathbf{y} + \Delta\mathbf{y}) = \mathbf{H}_{\gamma}(\mathbf{y} + \Delta\widehat{\mathbf{y}}_{\gamma})(\mathbf{y} + \Delta\mathbf{y}) - \gamma\eta_{\gamma}(\mathbf{y} + \Delta\mathbf{y}).$$

If the increment of $\mathbf{y}$ is small enough, e.g. $|\Delta\mathbf{y}| < \varepsilon$, Zou et al. (2007) showed that for Lasso the projection matrix $\mathbf{H}_{\gamma}$ and the function η_{γ} remain constant. Indeed, if γ is not a transition

point, small perturbations of $\mathbf{y}$ does not affect neither $\mathbf{H}_\gamma$ nor η_γ. In our case, instead, we have that $\mathbf{H}_\gamma(\mathbf{y}+\Delta\mathbf{y}) = \mathbf{H}_\gamma(\mathbf{y})$ but $\eta_\gamma(\mathbf{y}+\Delta\mathbf{y}) \neq \eta_\gamma(\mathbf{y})$, because $\mathbf{W}_\mathcal{A}(\mathbf{y}+\Delta\mathbf{y}) \neq \mathbf{W}_\mathcal{A}(\mathbf{y})$. Therefore

$$\widehat{\mathbf{y}}_\gamma(\mathbf{y}+\Delta\mathbf{y}) = \mathbf{H}_\gamma(\mathbf{y})(\mathbf{y}+\Delta\mathbf{y}) - \gamma\eta_\gamma(\mathbf{y}+\Delta\mathbf{y})$$

$$\frac{\widehat{\mathbf{y}}_\gamma(\mathbf{y}+\Delta\mathbf{y}) - \widehat{\mathbf{y}}_\gamma(\mathbf{y})}{\Delta\mathbf{y}} = \frac{\mathbf{H}_\gamma(\mathbf{y})\Delta\mathbf{y} - \gamma(\eta_\gamma(\mathbf{y}+\Delta\mathbf{y}) - \eta(\mathbf{y}))}{\Delta\mathbf{y}},$$

and

$$\frac{\partial\widehat{\mathbf{y}}_\gamma}{\partial\mathbf{y}} = \mathbf{H}_\gamma(\mathbf{y}) - \gamma\frac{\partial\eta_\gamma(\mathbf{y})}{\partial\mathbf{y}}. \tag{18}$$

By applying the trace operator, we have

$$\widehat{df}_\gamma = \mathrm{trace}\left(\frac{\partial\widehat{\mathbf{y}}_\gamma}{\partial\mathbf{y}}\right) = \mathrm{trace}\left(\mathbf{H}_\gamma(\mathbf{y}) - \gamma\frac{\partial\eta_\gamma(\mathbf{y})}{\partial\mathbf{y}}\right)$$

$$= \mathrm{trace}(\mathbf{X}_\mathcal{A}(\mathbf{X}_\mathcal{A}^\top\mathbf{X}_\mathcal{A})^{-1}\mathbf{X}_\mathcal{A}^\top) - \gamma\mathrm{trace}\left(\frac{\partial\mathbf{P}_\mathcal{A}\mathbf{W}_\mathcal{A}\mathrm{sgn}(\widehat{\boldsymbol{\beta}}_\mathcal{A})}{\partial\mathbf{y}}\right),$$

where $\mathbf{P} = \mathbf{X}(\mathbf{X}^\top\mathbf{X})^{-1} \in \mathbb{R}^{n\times p}$ and $\mathbf{P}_\mathcal{A} = \mathbf{X}_\mathcal{A}(\mathbf{X}_\mathcal{A}^\top\mathbf{X}_\mathcal{A})^{-1} \in \mathbb{R}^{n\times|\mathcal{A}|}$. Then, direct application of Lemma 1 in the Supplementary Materials, yields to:

$$\widehat{df}_\gamma = |\mathcal{A}| - \gamma\mathrm{trace}\left(\sum_{j\in\mathcal{A}}\mathrm{sgn}(\widehat{\beta}_j)\mathrm{sgn}(\widehat{\beta}_j^{\mathsf{LS}})\frac{\partial w_j(z)}{\partial z}\bigg|_{z=\widehat{\beta}_j^{\mathsf{LS}}}\mathbf{p}_j\mathbf{p}_{\mathcal{A},\pi(j)}^\top\right)$$

$$= |\mathcal{A}| - \gamma\sum_{j\in\mathcal{A}}\mathrm{sgn}(\widehat{\beta}_j)\mathrm{sgn}(\widehat{\beta}_j^{\mathsf{LS}})\frac{\partial w_j(z)}{\partial z}\bigg|_{z=\widehat{\beta}_j^{\mathsf{LS}}}\mathrm{trace}(\mathbf{p}_j\mathbf{p}_{\mathcal{A},\pi(j)}^\top)$$

$$= |\mathcal{A}| - \gamma\sum_{j\in\mathcal{A}}\mathrm{sgn}(\widehat{\beta}_j)\mathrm{sgn}(\widehat{\beta}_j^{\mathsf{LS}})\frac{\partial w_j(z)}{\partial z}\bigg|_{z=\widehat{\beta}_j^{\mathsf{LS}}}\mathrm{trace}(\mathbf{p}_{\mathcal{A},\pi(j)}^\top\mathbf{p}_j),$$

where $\mathbf{p}_j$ and $\mathbf{p}_{\mathcal{A},\pi(j)}$ denote the j-th column of the matrix $\mathbf{P}$ and the $\pi(j)$-th column of the matrix $\mathbf{P}_\mathcal{A}$, respectively. Note that we can write $\mathbf{p}_j = \mathbf{P}\mathbf{e}_j$ and $\mathbf{p}_{\mathcal{A},\pi(j)} = \mathbf{P}_\mathcal{A}\mathbf{e}_{\pi(j)}$, where $\mathbf{e}_j$ denotes a column vector with one in position j and zeros elsewhere. Let $\mathbf{S}_\mathcal{A} \in \{0,1\}^{|\mathcal{A}|\times p}$ denote the selection matrix obtained from the identity matrix $\mathbf{I}_p$ by retaining only the rows corresponding to the index set $\mathcal{A}$, i.e. $\mathbf{S}_\mathcal{A} \equiv \mathbf{I}_{[\mathcal{A},]}$. Then $\mathbf{X}_\mathcal{A} = \mathbf{X}\mathbf{S}_\mathcal{A}^\top$ and $\mathbf{X}_\mathcal{A}^\top\mathbf{P}\mathbf{e}_j = \mathbf{X}_\mathcal{A}^\top\mathbf{X}(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{e}_j = \mathbf{S}_\mathcal{A}\mathbf{X}^\top\mathbf{X}(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{e}_j = \mathbf{S}_\mathcal{A}\mathbf{e}_j = \mathbf{e}_{\pi(j)}$. Therefore

$$\mathbf{p}_{\mathcal{A},\pi(j)}^\top\mathbf{p}_j = \mathbf{e}_{\pi(j)}^\top(\mathbf{X}_\mathcal{A}^\top\mathbf{X}_\mathcal{A})^{-1}\mathbf{X}_\mathcal{A}^\top\mathbf{X}(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{e}_j = \mathbf{e}_{\pi(j)}^\top(\mathbf{X}_\mathcal{A}^\top\mathbf{X}_\mathcal{A})^{-1}\mathbf{e}_{\pi(j)} = [(\mathbf{X}_\mathcal{A}^\top\mathbf{X}_\mathcal{A})^{-1}]_{\pi(j),\pi(j)},$$

and

$$\widehat{df}_\gamma = |\mathcal{A}| - \gamma\sum_{j\in\mathcal{A}}\mathrm{sgn}(\widehat{\beta}_j)\mathrm{sgn}(\widehat{\beta}_j^{\mathsf{LS}})\frac{\partial w_j(z)}{\partial z}\bigg|_{z=\widehat{\beta}_j^{\mathsf{LS}}}[(\mathbf{X}_\mathcal{A}^\top\mathbf{X}_\mathcal{A})^{-1}]_{\pi(j),\pi(j)},$$

to arrive to the statement of the theorem. In the orthogonal case $\mathrm{sgn}(\widehat{\beta}_j)\mathrm{sgn}(\widehat{\beta}_j^{\mathsf{LS}}) = 1$ and $(\mathbf{X}_\mathcal{A}^\top\mathbf{X}_\mathcal{A})^{-1}_{\pi(j),\pi(j)} = 1$ for each j, which simplifies the above result to

$$\widehat{df}_\gamma = |\mathcal{A}| - \gamma\sum_{j\in\mathcal{A}}\frac{\partial w_j(z)}{\partial z}\bigg|_{z=\widehat{\beta}_j^{\mathsf{LS}}}.$$

$\square$

Proof of Corollary 1. Under the setting of Theorem 1 and the orthonormal design assumption, we have that $\mathbf{H}_\gamma(\mathbf{y}) = \mathbf{X}_\mathcal{A}\mathbf{X}_\mathcal{A}^\top$, $\eta_\gamma(\mathbf{y}) = \mathbf{X}_\mathcal{A}\mathbf{W}_\mathcal{A}(\mathbf{y})\operatorname{sgn}(\widehat{\boldsymbol{\beta}}_\mathcal{A})$ and $\widehat{\boldsymbol{\beta}}^{\mathsf{LS}} = \mathbf{X}^\top\mathbf{y}$. Moreover, if the weights are chosen as the inverse of the absolute values of least squares estimates the matrix $\mathbf{W}$ is given by

$$\mathbf{W} = \operatorname{diag}\Big(\frac{1}{|\widehat{\boldsymbol{\beta}}^{\mathsf{LS}}|}\Big) = \operatorname{diag}\Big(\frac{1}{|\mathbf{X}^\top\mathbf{y}|}\Big),$$

with generic term being $w_{jj} = w_j(|\widehat{\beta}_j^{\mathsf{LS}}|) = 1/|\widehat{\beta}_j^{\mathsf{LS}}| = 1/|\mathbf{x}_j^\top\mathbf{y}|$. By applying the result of Theorem 1 in the orthonormal case, we have

$$\frac{\partial w_j(z)}{\partial z}\Big|_{z=\widehat{\beta}_j^{\mathsf{LS}}} = \frac{\partial}{\partial z}\Big(\frac{1}{z}\Big)\Big|_{z=\widehat{\beta}_j^{\mathsf{LS}}} = -\frac{1}{z^2}\Big|_{z=\widehat{\beta}_j^{\mathsf{LS}}} = -\frac{1}{(\widehat{\beta}_j^{\mathsf{LS}})^2},$$

which concludes the proof. $\qquad\square$

Proof of Corollary 2. Under the setting of Theorem 1, we have $\widehat{\boldsymbol{\beta}}^{\mathsf{LS}} = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}$ and

$$\mathbf{W} = \operatorname{diag}\Big(\frac{1}{|\widehat{\boldsymbol{\beta}}^{\mathsf{LS}}|}\Big) = \operatorname{diag}\Big(\frac{1}{|(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}|}\Big),$$

with generic term being $w_{jj} = w_j(|\widehat{\beta}_j^{\mathsf{LS}}|) = 1/|\widehat{\beta}_j^{\mathsf{LS}}| = 1/|\mathbf{p}_j^\top\mathbf{y}|$, where $\mathbf{p}_j \in \mathbb{R}^n$ is the j-th column of $\mathbf{P} = \mathbf{X}(\mathbf{X}^\top\mathbf{X})^{-1} \in \mathbb{R}^{n\times p}$. By applying the result of Theorem 1 in the non-orthonormal case, we have

$$\frac{\partial w_j(z)}{\partial z}\Big|_{z=\widehat{\beta}_j^{\mathsf{LS}}} = \frac{\partial}{\partial z}\Big(\frac{1}{z}\Big)\Big|_{z=\widehat{\beta}_j^{\mathsf{LS}}} = -\frac{1}{z^2}\Big|_{z=\widehat{\beta}_j^{\mathsf{LS}}} = -\frac{1}{(\widehat{\beta}_j^{\mathsf{LS}})^2},$$

which concludes the proof. $\qquad\square$

Proof of corollary 3. Define a mapping $\pi : \mathcal{A} \to \{1, 2, \ldots, |\mathcal{A}|\}$ such that for each $j \in \mathcal{A}$, $\pi(j) = i$ if $\mathcal{A}_i = j$. We first prove that $b_l > 0$ for each l and then that $b_l > b_{l+1}$ for each l. To prove the first inequality, note that the estimated degrees of freedom are given by a linear function $|\mathcal{A}| + b_l\gamma$, where the slope b_l is, by Theorem 1, equal to:

$$b_l = -\sum_{j\in\mathcal{A}} \operatorname{sgn}(\widehat{\beta}_j)\operatorname{sgn}(\widehat{\beta}_j^{\mathsf{LS}})\frac{\partial w(z)}{\partial z}\Big|_{x=\widehat{\beta}_j^{\mathsf{LS}}}[(\mathbf{X}_\mathcal{A}^\top\mathbf{X}_\mathcal{A})^{-1}]_{\pi(j),\pi(j)}.$$

This quantity is strictly positive because by theorem's assumptions we must have $\mathcal{A} \neq \emptyset$, signs concordance and $w'(|\beta_j^{\mathsf{LS}}|) < 0$, and $[(\mathbf{X}_\mathcal{A}^\top\mathbf{X}_\mathcal{A})^{-1}]_{\pi(j),\pi(j)} > 0$.

To prove the second inequality, define with $\mathcal{A}_l$ the active set for $\gamma \in (\gamma_l, \gamma_{l+1})$ and with $\mathcal{A}_{l+1}$ the active set for $\gamma \in (\gamma_{l+1}, \gamma_{l+2})$. Under the assumptions of the Corollary, we have $\mathcal{A}_{l+1} \subset \mathcal{A}_l$. Assume without loss of generality that moving from $\mathcal{A}_l$ to $\mathcal{A}_{l+1}$ the k-th coefficient leaves the active set i.e., $\mathcal{A}_l \setminus \mathcal{A}_{l+1} = \beta_k$. Then,

$$\begin{aligned}
b_l &= -\sum_{j\in\mathcal{A}_l} \operatorname{sgn}(\widehat{\beta}_j)\operatorname{sgn}(\widehat{\beta}_j^{\mathsf{LS}})\frac{\partial w(z)}{\partial z}\Big|_{x=\widehat{\beta}_j^{\mathsf{LS}}}[(\mathbf{X}_\mathcal{A}^\top\mathbf{X}_\mathcal{A})^{-1}]_{\pi(j),\pi(j)} \\
&= -\sum_{j\in\mathcal{A}_{l+1}} \operatorname{sgn}(\widehat{\beta}_j)\operatorname{sgn}(\widehat{\beta}_j^{\mathsf{LS}})\frac{\partial w(z)}{\partial z}\Big|_{x=\widehat{\beta}_j^{\mathsf{LS}}}[(\mathbf{X}_\mathcal{A}^\top\mathbf{X}_\mathcal{A})^{-1}]_{\pi(j),\pi(j)} \\
&\qquad - \operatorname{sgn}(\widehat{\beta}_k)\operatorname{sgn}(\widehat{\beta}_k^{\mathsf{LS}})\frac{\partial w(z)}{\partial z}\Big|_{x=\widehat{\beta}_k^{\mathsf{LS}}}[(\mathbf{X}_\mathcal{A}^\top\mathbf{X}_\mathcal{A})^{-1}]_{\pi(k),\pi(k)} = b_{l+1} + c,
\end{aligned}$$

with $c > 0$, concluding the proof. $\qquad\square$

of Theorem 2. Let $\mathbf{W} = \mathrm{diag}(w_1, \ldots, w_G) \in \mathbb{S}_{++}^G$. The first order conditions for the problem in Equation (9) are represented by

$$-\mathbf{X}_{\mathcal{A}_G}^\top(\mathbf{y} - \mathbf{X}_{\mathcal{A}_G}\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}) + \gamma\widetilde{\boldsymbol{\beta}}_{\mathcal{A}_G} = \mathbf{0},$$

where $\mathbf{X}_{\mathcal{A}_G}$ and $\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}$ are restricted to the active set $\mathcal{A}_G$, and $\widetilde{\boldsymbol{\beta}}_{\mathcal{A}_G}$ is a column vector whose entries are $\left[w_g\widehat{\boldsymbol{\beta}}_g/\|\widehat{\boldsymbol{\beta}}_g\|_2\right]_{g \in \mathcal{A}_G}$. Similarly to Lasso and Adaptive Lasso, by manipulating terms recalling the orthonormal design assumption, we arrive to the following expression:

$$\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G} = (\mathbf{X}_{\mathcal{A}_G}^\top\mathbf{X}_{\mathcal{A}_G})^{-1}(\mathbf{X}_{\mathcal{A}_G}^\top\mathbf{y} - \gamma\widetilde{\boldsymbol{\beta}}_{\mathcal{A}_G}) = \mathbf{X}_{\mathcal{A}_G}^\top\mathbf{y} - \gamma\widetilde{\boldsymbol{\beta}}_{\mathcal{A}_G},$$

and denoting

$$\mathbf{H}_\gamma(\mathbf{y}) = \mathbf{X}_{\mathcal{A}_G}\mathbf{X}_{\mathcal{A}_G}^\top, \qquad \eta_\gamma(\mathbf{y}) = \mathbf{X}_{\mathcal{A}_G}\widetilde{\boldsymbol{\beta}}_{\mathcal{A}_G},$$

we get the expression linking $\widehat{\mathbf{y}}_\gamma$ and $\mathbf{y}$

$$\widehat{\mathbf{y}}_\gamma = \mathbf{X}\widehat{\boldsymbol{\beta}} = \mathbf{H}_\gamma(\mathbf{y})\mathbf{y} - \gamma\eta_\gamma(\mathbf{y}).$$

Considering the increments $\mathbf{y} + \Delta\mathbf{y}$, we have again $\eta_\gamma(\mathbf{y} + \Delta\mathbf{y}) \neq \eta_\gamma(\mathbf{y})$ and arrive again at Equation (18). However, for Group Lasso is not easy to work with this expression directly, as η_γ is function of $\mathbf{y}$ in an indirect way, since the dependence on $\mathbf{y}$ only appears through $\widehat{\boldsymbol{\beta}}$. Despite that, exploiting the chain rule, we insert $\partial\widehat{\mathbf{y}}_\gamma/\partial\mathbf{y}$ in the right side of the equation allowing us to write

$$\frac{\partial\widehat{\mathbf{y}}_\gamma}{\partial\mathbf{y}} = \mathbf{H}_\gamma(\mathbf{y}) - \gamma\frac{\partial\eta_\gamma(\mathbf{y})}{\partial\widehat{\mathbf{y}}}\frac{\partial\widehat{\mathbf{y}}_\gamma}{\partial\mathbf{y}},$$

and, by isolating the quantity of interest, obtaining

$$\frac{\partial\widehat{\mathbf{y}}_\gamma}{\partial\mathbf{y}} = \left(\mathbf{I}_n + \gamma\frac{\partial\eta_\gamma(\mathbf{y})}{\partial\widehat{\mathbf{y}}}\right)^{-1}\mathbf{H}_\gamma(\mathbf{y}). \tag{19}$$

In order to compute $\partial\eta_\gamma(\mathbf{y})/\partial\widehat{\mathbf{y}}$ we make use again of the chain rule:

$$\frac{\partial\eta_\gamma(\mathbf{y})}{\partial\widehat{\mathbf{y}}} = \frac{\partial\eta_\gamma(\mathbf{y})}{\partial\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}}\frac{\partial\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}}{\partial\widehat{\mathbf{y}}}.$$

By applying Lemma 2 in the Supplementary Materials, to the former term, we obtain:

$$\frac{\partial\eta_\gamma(\mathbf{y})}{\partial\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}} = \begin{bmatrix}\frac{\partial\eta_\gamma(\mathbf{y})}{\partial\widehat{\boldsymbol{\beta}}_1} & \cdots & \frac{\partial\eta_\gamma(\mathbf{y})}{\partial\widehat{\boldsymbol{\beta}}_G}\end{bmatrix} = \begin{bmatrix}\frac{\partial}{\partial\widehat{\boldsymbol{\beta}}_1}\left(\frac{w_1\mathbf{X}_1\widehat{\boldsymbol{\beta}}_1}{\|\widehat{\boldsymbol{\beta}}_1\|_2}\right) & \cdots & \frac{\partial}{\partial\widehat{\boldsymbol{\beta}}_G}\left(\frac{w_G\mathbf{X}_G\widehat{\boldsymbol{\beta}}_G}{\|\widehat{\boldsymbol{\beta}}_G\|_2}\right)\end{bmatrix}$$

$$= \begin{bmatrix}w_1\mathbf{X}_1\frac{\partial}{\partial\widehat{\boldsymbol{\beta}}_1}\left(\frac{\widehat{\boldsymbol{\beta}}_1}{\|\widehat{\boldsymbol{\beta}}_1\|_2}\right) & \cdots & w_G\mathbf{X}_G\frac{\partial}{\partial\widehat{\boldsymbol{\beta}}_G}\left(\frac{\widehat{\boldsymbol{\beta}}_G}{\|\widehat{\boldsymbol{\beta}}_G\|_2}\right)\end{bmatrix}$$

$$= \begin{bmatrix}w_1\mathbf{X}_1\left(\frac{\mathbf{I}_p}{\|\widehat{\boldsymbol{\beta}}_1\|_2} - \frac{\widehat{\boldsymbol{\beta}}_1\widehat{\boldsymbol{\beta}}_1^\top}{\|\widehat{\boldsymbol{\beta}}_1\|_2^3}\right) & \cdots & w_G\mathbf{X}_G\left(\frac{\mathbf{I}_p}{\|\widehat{\boldsymbol{\beta}}_G\|_2} - \frac{\widehat{\boldsymbol{\beta}}_G\widehat{\boldsymbol{\beta}}_G^\top}{\|\widehat{\boldsymbol{\beta}}_G\|_2^3}\right)\end{bmatrix},$$

and, by defining

$$\boldsymbol{\Pi}_g = w_g\left(\frac{\mathbf{I}_p}{\|\widehat{\boldsymbol{\beta}}_g\|_2} - \frac{\widehat{\boldsymbol{\beta}}_g\widehat{\boldsymbol{\beta}}_g^\top}{\|\widehat{\boldsymbol{\beta}}_g\|_2^3}\right) \quad \text{and} \quad \boldsymbol{\Pi}_{\mathcal{A}_G} = \mathrm{blockdiag}(\boldsymbol{\Pi}_1, \ldots, \boldsymbol{\Pi}_G), \tag{20}$$

we get

$$\frac{\partial\eta_\gamma(\mathbf{y})}{\partial\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}} = \begin{bmatrix}\mathbf{X}_1\boldsymbol{\Pi}_1 & \cdots & \mathbf{X}_g\boldsymbol{\Pi}_g & \cdots & \mathbf{X}_G\boldsymbol{\Pi}_G\end{bmatrix}$$

$$= \begin{bmatrix}\mathbf{X}_1 & \cdots & \mathbf{X}_g & \cdots & \mathbf{X}_G\end{bmatrix}\begin{bmatrix}\boldsymbol{\Pi}_1 & \cdots & 0 & \cdots & 0 \\ 0 & \cdots & \boldsymbol{\Pi}_g & \cdots & 0 \\ 0 & \cdots & 0 & \cdots & \boldsymbol{\Pi}_G\end{bmatrix} = \mathbf{X}_{\mathcal{A}_G}\boldsymbol{\Pi}_{\mathcal{A}_G}.$$

For the latter, since $\widehat{\mathbf{y}} = \mathbf{X}_{\mathcal{A}_G}\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}$, we have

$$\frac{\partial\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}}{\partial\widehat{\mathbf{y}}} = \left(\frac{\partial\widehat{\mathbf{y}}}{\partial\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}}\right)^{-1} = \left(\frac{\partial\mathbf{X}_{\mathcal{A}_G}\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}}{\partial\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}}\right)^{-1} = \mathbf{X}_{\mathcal{A}_G}^{-} = \mathbf{X}_{\mathcal{A}_G}^{\top}.$$

The final expression for $\partial\eta_\gamma(\mathbf{y})/\partial\widehat{\mathbf{y}}$ is therefore

$$\frac{\partial\eta_\gamma(\mathbf{y})}{\partial\widehat{\mathbf{y}}} = \frac{\partial\eta_\gamma(\mathbf{y})}{\partial\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}}\frac{\partial\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}}{\partial\widehat{\mathbf{y}}} = \mathbf{X}_{\mathcal{A}_G}\boldsymbol{\Pi}_{\mathcal{A}_G}\mathbf{X}_{\mathcal{A}_G}^{\top}.$$

To compute degrees of freedom, from Equation (19), we write

$$\widehat{df}_\gamma = \mathrm{trace}\left(\frac{\partial\widehat{\mathbf{y}}_\gamma}{\partial\mathbf{y}}\right) = \mathrm{trace}\left\{\left(\mathbf{I}_n + \gamma\frac{\partial\eta_\gamma(\mathbf{y})}{\partial\widehat{\mathbf{y}}}\right)^{-1}\mathbf{H}_\gamma(\mathbf{y})\right\}$$

$$= \mathrm{trace}\left\{(\mathbf{I}_n + \gamma\mathbf{X}_{\mathcal{A}_G}\boldsymbol{\Pi}_{\mathcal{A}_G}\mathbf{X}_{\mathcal{A}_G}^{\top})^{-1}\mathbf{X}_{\mathcal{A}_G}\mathbf{X}_{\mathcal{A}_G}^{\top}\right\},$$

completing the proof. $\qquad\square$

Proof of Theorem 3. The proof follows a structure similar to that in the previous one. When the design matrix is not orthogonal, we have $\mathbf{H}_\gamma(\mathbf{y}) = \mathbf{X}_{\mathcal{A}_G}(\mathbf{X}_{\mathcal{A}_G}^{\top}\mathbf{X}_{\mathcal{A}_G})^{-1}\mathbf{X}_{\mathcal{A}_G}^{\top}$ and $\eta_\gamma(\mathbf{y}) = \mathbf{X}_{\mathcal{A}_G}\left(\mathbf{X}_{\mathcal{A}_G}^{\top}\mathbf{X}_{\mathcal{A}_G}\right)^{-1}\widetilde{\boldsymbol{\beta}}_{\mathcal{A}_G}$. For convenience, define $\mathbf{P} = \mathbf{X}_{\mathcal{A}_G}(\mathbf{X}_{\mathcal{A}_G}^{\top}\mathbf{X}_{\mathcal{A}_G})^{-1}$ and $\mathbf{P}_g$ the generic g-th column of $\mathbf{P}$. Consequently, we can rewrite:

$$\frac{\partial\eta_\gamma(\mathbf{y})}{\partial\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}} = \begin{bmatrix}\frac{\partial\eta_\gamma(\mathbf{y})}{\partial\widehat{\boldsymbol{\beta}}_1} & \cdots & \frac{\partial\eta_\gamma(\mathbf{y})}{\partial\widehat{\boldsymbol{\beta}}_G}\end{bmatrix} = \begin{bmatrix}\frac{\partial}{\partial\widehat{\boldsymbol{\beta}}_1}\left(\frac{w_1\mathbf{P}_1\widehat{\boldsymbol{\beta}}_1}{\|\widehat{\boldsymbol{\beta}}_1\|_2}\right) & \cdots & \frac{\partial}{\partial\widehat{\boldsymbol{\beta}}_G}\left(\frac{w_G\mathbf{P}_G\widehat{\boldsymbol{\beta}}_G}{\|\widehat{\boldsymbol{\beta}}_G\|_2}\right)\end{bmatrix}$$

$$= \begin{bmatrix}w_1\mathbf{P}_1\frac{\partial}{\partial\widehat{\boldsymbol{\beta}}_1}\left(\frac{\widehat{\boldsymbol{\beta}}_1}{\|\widehat{\boldsymbol{\beta}}_1\|_2}\right) & \cdots & w_G\mathbf{P}_G\frac{\partial}{\partial\widehat{\boldsymbol{\beta}}_G}\left(\frac{\widehat{\boldsymbol{\beta}}_G}{\|\widehat{\boldsymbol{\beta}}_G\|_2}\right)\end{bmatrix}$$

$$= \begin{bmatrix}w_1\mathbf{P}_1\left(\frac{\mathbf{I}_p}{\|\widehat{\boldsymbol{\beta}}_1\|_2} - \frac{\widehat{\boldsymbol{\beta}}_1\widehat{\boldsymbol{\beta}}_1^{\top}}{\|\widehat{\boldsymbol{\beta}}_1\|_2^3}\right) & \cdots & w_G\mathbf{P}_G\left(\frac{\mathbf{I}_p}{\|\widehat{\boldsymbol{\beta}}_G\|_2} - \frac{\widehat{\boldsymbol{\beta}}_G\widehat{\boldsymbol{\beta}}_G^{\top}}{\|\widehat{\boldsymbol{\beta}}_G\|_2^3}\right)\end{bmatrix},$$

from which we get

$$\frac{\partial\eta_\gamma(\mathbf{y})}{\partial\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}} = \begin{bmatrix}\mathbf{P}_1\boldsymbol{\Pi}_1 & \cdots & \mathbf{P}_g\boldsymbol{\Pi}_g & \cdots & \mathbf{P}_G\boldsymbol{\Pi}_G\end{bmatrix}$$

$$= \begin{bmatrix}\mathbf{P}_1 & \cdots & \mathbf{P}_g & \cdots & \mathbf{P}_G\end{bmatrix}\begin{bmatrix}\boldsymbol{\Pi}_1 & \cdots & 0 & \cdots & 0 \\ 0 & \cdots & \boldsymbol{\Pi}_g & \cdots & 0 \\ 0 & \cdots & 0 & \cdots & \boldsymbol{\Pi}_G\end{bmatrix}$$

$$= \mathbf{P}\boldsymbol{\Pi}_{\mathcal{A}_G} = \mathbf{X}_{\mathcal{A}_G}(\mathbf{X}_{\mathcal{A}_G}^{\top}\mathbf{X}_{\mathcal{A}_G})^{-1}\boldsymbol{\Pi}_{\mathcal{A}_G}.$$

For the latter, since $\widehat{\mathbf{y}} = \mathbf{X}_{\mathcal{A}_G}\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}$, we have

$$\frac{\partial\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}}{\partial\widehat{\mathbf{y}}} = \left(\frac{\partial\widehat{\mathbf{y}}}{\partial\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}}\right)^{-1} = \left(\frac{\partial\mathbf{X}_{\mathcal{A}_G}\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}}{\partial\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}}\right)^{-1} = \mathbf{X}_{\mathcal{A}_G}^{-} = (\mathbf{X}_{\mathcal{A}_G}^{\top}\mathbf{X}_{\mathcal{A}_G})^{-1}\mathbf{X}_{\mathcal{A}_G}^{\top}.$$

The final expression for the derivative $\partial\eta_\gamma(\mathbf{y})/\partial\widehat{\mathbf{y}}$, is therefore

$$\frac{\partial\eta_\gamma(\mathbf{y})}{\partial\widehat{\mathbf{y}}} = \frac{\partial\eta_\gamma(\mathbf{y})}{\partial\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}}\frac{\partial\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}}{\partial\widehat{\mathbf{y}}} = \mathbf{X}_{\mathcal{A}_G}(\mathbf{X}_{\mathcal{A}_G}^{\top}\mathbf{X}_{\mathcal{A}_G})^{-1}\boldsymbol{\Pi}_{\mathcal{A}_G}(\mathbf{X}_{\mathcal{A}_G}^{\top}\mathbf{X}_{\mathcal{A}_G})^{-1}\mathbf{X}_{\mathcal{A}_G}^{\top}.$$

To compute the degrees of freedom, we use Equation (19) and write:

$$\widehat{df}_\gamma = \text{trace}\left(\frac{\partial \widehat{\mathbf{y}}_\gamma}{\partial \mathbf{y}}\right) = \text{trace}\left\{\left(\mathbf{I}_n + \gamma \frac{\partial \eta_\gamma(\mathbf{y})}{\partial \widehat{\mathbf{y}}}\right)^{-1} \mathbf{H}_\gamma(\mathbf{y})\right\}$$

$$= \text{trace}\left\{\left(\mathbf{I}_n + \gamma \mathbf{X}_{\mathcal{A}_G}(\mathbf{X}_{\mathcal{A}_G}^\top \mathbf{X}_{\mathcal{A}_G})^{-1}\mathbf{\Pi}_{\mathcal{A}_G}(\mathbf{X}_{\mathcal{A}_G}^\top \mathbf{X}_{\mathcal{A}_G})^{-1}\mathbf{X}_{\mathcal{A}_G}^\top\right)^{-1} \mathbf{X}_{\mathcal{A}_G}(\mathbf{X}_{\mathcal{A}_G}^\top \mathbf{X}_{\mathcal{A}_G})^{-1}\mathbf{X}_{\mathcal{A}_G}^\top\right\},$$

which completes the proof. □

Proof of corollary 4. We begin by noting that both the matrices $\mathbf{A}$ and $\mathbf{B}$ introduced in Theorems 2 and 3 are positive semidefinite. The matrix $\mathbf{A}$ has its first $|\mathcal{A}_p|$ eigenvalues equal to 1, with all remaining eigenvalues equal to 0. The matrix $\mathbf{B}$ is also positive semidefinite, since each component matrix $\mathbf{\Pi}_g$ is. In fact, since $w_g/\|\boldsymbol{\beta}_g\|_2 > 0$, and the matrix $\mathbf{I}_{n_g} - \boldsymbol{\beta}_g \boldsymbol{\beta}_g^\top/\|\boldsymbol{\beta}_g\|_2^2$ has $n_g - 1$ eigenvalues equal to 1 and one equal to 0, each $\mathbf{\Pi}_g$ inherits this semi-definiteness. When $\mathbf{X}$ is orthonormal, the eigenvalues of $\mathbf{B}$ are

$$\lambda(\mathbf{B}) = \left(\bigcup_{g \in \mathcal{A}} \Big\{\underbrace{\frac{w_g}{\|\widehat{\boldsymbol{\beta}}_g\|_2}, \dots, \frac{w_g}{\|\widehat{\boldsymbol{\beta}}_g\|_2}}_{n_g-1}, 0\Big\}, \underbrace{0, \dots, 0}_{n-|\mathcal{A}_p|}\right),$$

for a total of $|\mathcal{A}_p| - |\mathcal{A}_G|$ eigenvalues greater than zero and the remaining eigenvalues equal to zero. In the non orthonormal case, the expression of the eigenvalues of $\mathbf{B}$ is not known, but we still have $|\mathcal{A}_p| - |\mathcal{A}_G|$ eigenvalues greater than zero and the remaining eigenvalues equal to zero. When the design is orthonormal,

$$\text{trace}((\mathbf{I}_n + \gamma \mathbf{B})^{-1}\mathbf{A}) = \sum_{i=1}^{n} \frac{\lambda_i^A}{1 + \gamma \lambda_i^B}, \tag{21}$$

where λ_i^A and λ_i^B are the eigenvalues of $\mathbf{A}$ and $\mathbf{B}$, respectively. It is straightforward to prove that Equation (21) is a continuous function of γ. Given the eigenstructure of the two matrices, the first $|\mathcal{A}_p| - |\mathcal{A}_G|$ eigenvalues of $\mathbf{A}$ are shrinked by the positive amount $1 + \gamma \lambda_i^B$, the following $|\mathcal{A}_G|$ eigenvalues of $\mathbf{A}$ remain equal to 1 because the corresponding λ_i^B is zero, and the remaining eigenvalues are zero. We can thus conclude that

$$|\mathcal{A}_G| \le \text{trace}((\mathbf{I}_n + \gamma \mathbf{B})^{-1}\mathbf{A}) \le \text{trace}(\mathbf{A}) = |\mathcal{A}_p|.$$

For the non orthonormal design, we apply Von Neumann's trace inequality:

$$|\mathcal{A}_G| \le \sum_{i=1}^{n} \frac{\lambda_i^A}{1 + \gamma \lambda_i^B} \le \text{trace}((\mathbf{I}_n + \gamma \mathbf{B})^{-1}\mathbf{A}) \le \sum_{i=1}^{n} \frac{\lambda_i^A}{1 + \gamma \lambda_{n-i+1}^B} \le \sum_{i=1}^{n} \lambda_i^A = |\mathcal{A}_p|, \tag{22}$$

thus the degrees of freedom of Group Lasso are always lower than the number of active *variables* $|\mathcal{A}_p|$ and greater than the number of active *groups* $|\mathcal{A}_G|$. The equality in the previous expression is achieved if $\gamma = 0$ (in which case $\widehat{df}_\gamma = p$), if $|\mathcal{A}_p| = |\mathcal{A}_G| = 0$ (in which case $\widehat{df}_\gamma = 0$) or if $n_g = 1$ (in which case Lasso is being fitted). □

Proof of Theorem 4. Taking the derivative of $\widehat{df}_\gamma$ with respect to $\gamma > 0$, we have

$$\frac{\mathrm{d}\widehat{df}_\gamma}{\mathrm{d}\gamma} = \frac{\mathrm{d}}{\mathrm{d}\gamma}\text{trace}\left[(\mathbf{I}_n + \gamma \mathbf{B})^{-1}\mathbf{A}\right]$$

$$= -\text{trace}\left[\left(\mathbf{\Pi}_{\mathcal{A}_G} + \gamma \frac{\mathrm{d}\mathbf{\Pi}_{\mathcal{A}_G}}{\mathrm{d}\gamma}\right)\mathbf{M}_{\mathcal{A}_G}^\top (\mathbf{I}_n + \gamma \mathbf{B})^{-1}\mathbf{A}(\mathbf{I}_n + \gamma \mathbf{B})^{-1}\mathbf{M}_{\mathcal{A}_G}\right],$$

where, to get the previous result, we used the fact that

$$\frac{\mathrm{d}\mathbf{B}}{\mathrm{d}\gamma} = \mathbf{M}_{\mathcal{A}_G} \frac{\mathrm{d}\mathbf{\Pi}_{\mathcal{A}_G}}{\mathrm{d}\gamma} \mathbf{M}_{\mathcal{A}_G}^\top.$$

For the derivative $\mathrm{d}\widehat{df}_\gamma/d\gamma$ to be negative the trace should be positive. Note that as in Equation (22), the matrices $\mathbf{I}_n + \gamma\mathbf{B}$ and $\mathbf{A}$ have non-negative eigenvalues, therefore it remains to prove that all the eigenvalues of

$$\mathbf{B} + \gamma\frac{\mathrm{d}\mathbf{B}}{\mathrm{d}\gamma} = \mathbf{M}_{\mathcal{A}_G}\left(\mathbf{\Pi}_{\mathcal{A}_G} + \gamma\frac{\mathrm{d}\mathbf{\Pi}_{\mathcal{A}_G}}{\mathrm{d}\gamma}\right)\mathbf{M}_{\mathcal{A}_G}^\top,$$

are non-negative. Since $\mathbf{\Pi}_{\mathcal{A}_G} + \gamma\mathrm{d}\mathbf{\Pi}_{\mathcal{A}_G}/\mathrm{d}\gamma$ is positive semidefinite by assumption, we have the proof. $\qquad\square$

Proof of Theorem 5. Consider the derivative of $\mathbf{\Pi}_{\mathcal{A}_G}$ wrt γ. Since $\mathbf{\Pi}_{\mathcal{A}_G}$ is block-diagonal with blocks defined in Equation (20), then the derivative can be computed blockwise:

$$\frac{\mathrm{d}\mathbf{\Pi}_{\mathcal{A}_G}}{\mathrm{d}\gamma} = \mathrm{blockdiag}\Big(\frac{\mathrm{d}\mathbf{\Pi}_1}{\mathrm{d}\gamma}, \ldots, \frac{\mathrm{d}\mathbf{\Pi}_G}{\mathrm{d}\gamma}\Big).$$

Applying the chain rule for the derivative, and defining $r_g = \|\widehat{\boldsymbol{\beta}}_g\|_2$, we have

$$\frac{\mathrm{d}\mathbf{\Pi}_g}{\mathrm{d}\gamma} = -\frac{w_g}{r_g^2}\frac{\mathrm{d}r_g}{\mathrm{d}\gamma}\Big(\mathbf{I}_{n_g} - \frac{3}{r_g^2}\widehat{\boldsymbol{\beta}}_g\widehat{\boldsymbol{\beta}}_g^\top\Big) - \frac{w_g}{r_g^3}\Big(\frac{\mathrm{d}\widehat{\boldsymbol{\beta}}_g}{\mathrm{d}\gamma}\widehat{\boldsymbol{\beta}}_g^\top + \widehat{\boldsymbol{\beta}}_g\frac{\mathrm{d}\widehat{\boldsymbol{\beta}}_g}{\mathrm{d}\gamma}^\top\Big), \quad g \in \mathcal{A}_G, \tag{23}$$

$\frac{\mathrm{d}\widehat{\boldsymbol{\beta}}_g}{\mathrm{d}\gamma} = \frac{\mathrm{d}\widehat{\boldsymbol{\beta}}_g}{\mathrm{d}\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}}\frac{\mathrm{d}\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}}{\mathrm{d}\gamma} = \mathbf{S}_g\frac{\mathrm{d}\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}}{\mathrm{d}\gamma}$, and $\mathbf{S}_g \in \{0,1\}^{n_g \times |\mathcal{A}_G|}$ denotes the selection matrix obtained from the identity matrix $\mathbf{I}_{|\mathcal{A}_G|}$ by retaining only the rows corresponding to the g-th group. To compute the derivative $\frac{\mathrm{d}\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}}{\mathrm{d}\gamma}$, we apply the implicit function theorem to the equation:

$$F(\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}, \gamma) = -\mathbf{X}_{\mathcal{A}_G}^\top\Big(\mathbf{y} - \mathbf{X}_{\mathcal{A}_G}\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}\Big) + \gamma\widetilde{\boldsymbol{\beta}}_{\mathcal{A}_G} = \mathbf{0}.$$

Differentiating $F(\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}, \gamma)$ with respect to γ and solving for $\frac{\mathrm{d}\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}}{\mathrm{d}\gamma}$ gives:

$$\frac{\mathrm{d}\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}}{\mathrm{d}\gamma} = -\left(\frac{\partial F}{\partial\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}}\right)^{-1}\frac{\partial F}{\partial\gamma} \in \mathbb{R}^{|\mathcal{A}_G|}, \tag{24}$$

where

$$\frac{\partial F}{\partial\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}} = \mathbf{X}_{\mathcal{A}_G}^\top\mathbf{X}_{\mathcal{A}_G} + \gamma\mathbf{\Pi}_{\mathcal{A}_G} \in \mathbb{S}_+^{|\mathcal{A}_G|}, \quad \frac{\partial F}{\partial\gamma} = \widetilde{\boldsymbol{\beta}}_{\mathcal{A}_G} \in \mathbb{R}^{|\mathcal{A}_G|},$$

and, substituting in Equation (24), we get the final expression for the derivative:

$$\frac{\mathrm{d}\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}}{\mathrm{d}\gamma} = -\Big(\mathbf{X}_{\mathcal{A}_G}^\top\mathbf{X}_{\mathcal{A}_G} + \gamma\mathbf{\Pi}_{\mathcal{A}_G}\Big)^{-1}\widetilde{\boldsymbol{\beta}}_{\mathcal{A}_G} = -\mathbf{R}_{\mathcal{A}_G}\widetilde{\boldsymbol{\beta}}_{\mathcal{A}_G} = -\mathbf{R}_{\mathcal{A}_G}^\star\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G} \in \mathbb{R}^{|\mathcal{A}_G|}. \tag{25}$$

where $\mathbf{R}_{\mathcal{A}_G}^\star = \mathbf{R}_{\mathcal{A}_G}\mathbf{W}_{\mathcal{A}_G}, \mathbf{W}_{\mathcal{A}_G} = \mathrm{diag}\Big\{\frac{w_g}{\|\widehat{\boldsymbol{\beta}}_g\|_2}\boldsymbol{\iota}_{n_g}\Big\}_{g\in\mathcal{A}_G}$. Moreover, letting $r_{\mathcal{A}_G} = \|\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}\|_2$ and $r_g = \|\widehat{\boldsymbol{\beta}}_g\|_2$, which are functions of γ, we aim to compute their derivative with respect to γ. Using the chain rule, we obtain the following:

$$\frac{\mathrm{d}r_{\mathcal{A}_G}}{\mathrm{d}\gamma} = \frac{\mathrm{d}}{\mathrm{d}\gamma}\Big(\|\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}\|_2\Big) = \frac{1}{\|\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}\|_2}\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}^\top\frac{\mathrm{d}\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}}{\mathrm{d}\gamma}.$$

Substituting the expression for $\frac{\mathrm{d}\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}}{\mathrm{d}\gamma}$ from Equation (25), we get:

$$\frac{\mathrm{d}r_{\mathcal{A}_G}}{\mathrm{d}\gamma} = \frac{1}{\|\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}\|_2}\left(-\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}^\top \mathbf{R}_{\mathcal{A}_G}\widetilde{\boldsymbol{\beta}}_{\mathcal{A}_G}\right) = -\frac{\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}^\top \mathbf{R}_{\mathcal{A}_G}\widetilde{\boldsymbol{\beta}}_{\mathcal{A}_G}}{\|\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}\|_2} = -\frac{\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}^\top \mathbf{R}_{\mathcal{A}_G}^\star\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}}{\|\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}\|_2},$$

and

$$\frac{\mathrm{d}r_g}{\mathrm{d}\gamma} = \frac{\mathrm{d}}{\mathrm{d}\gamma}\left(\|\widehat{\boldsymbol{\beta}}_g\|_2\right) = \frac{1}{\|\widehat{\boldsymbol{\beta}}_g\|_2}\widehat{\boldsymbol{\beta}}_g^\top \frac{\mathrm{d}\widehat{\boldsymbol{\beta}}_g}{\mathrm{d}\gamma} = -\frac{1}{\|\widehat{\boldsymbol{\beta}}_g\|_2}\widehat{\boldsymbol{\beta}}_g^\top \left[\mathbf{R}_{\mathcal{A}_G}^\star\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}\right]_g. \tag{26}$$

Substituting the expression for $\frac{\mathrm{d}\widehat{\boldsymbol{\beta}}_g}{\mathrm{d}\gamma}$ into Equation (23), we get:

$$\frac{\mathrm{d}\boldsymbol{\Pi}_g}{\mathrm{d}\gamma} = -\frac{w_g}{r_g^2}\frac{\mathrm{d}r_g}{\mathrm{d}\gamma}\left(\mathbf{I}_{n_g} - \frac{3}{r_g^2}\widehat{\boldsymbol{\beta}}_g\widehat{\boldsymbol{\beta}}_g^\top\right) + \frac{w_g}{r_g^3}\left(\left[\mathbf{R}_{\mathcal{A}_G}^\star\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}\right]_g\widehat{\boldsymbol{\beta}}_g^\top + \widehat{\boldsymbol{\beta}}_g\left[\mathbf{R}_{\mathcal{A}_G}^\star\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}\right]_g^\top\right). \tag{27}$$

We are interested in finding all the eigenvalues of the matrix $\boldsymbol{\Pi}_{\mathcal{A}_G} + \gamma\mathrm{d}\boldsymbol{\Pi}_{\mathcal{A}_G}/\mathrm{d}\gamma$. Let $\mathbf{u}_g = \widehat{\boldsymbol{\beta}}_g$, $\mathbf{v}_g = \left[\mathbf{R}_{\mathcal{A}_G}^\star\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}\right]_g$, the eigenvalues of the g-th block of $\boldsymbol{\Pi}_{\mathcal{A}_G} + \gamma\mathrm{d}\boldsymbol{\Pi}_{\mathcal{A}_G}/\mathrm{d}\gamma$ can be calculated using Lemma 3 in the Supplementary Materials. Specifically

$$\lambda_{1,g} = \frac{1}{2}(2a_g + b_g\|\mathbf{u}_g\|_2^2 + 2c_g\mathbf{v}_g^\top\mathbf{u}_g) + \frac{1}{2}\sqrt{\Delta_g},$$

$$\lambda_{2,g} = a_g, \qquad \text{with multiplicity } n_g - 2,$$

$$\lambda_{3,g} = \frac{1}{2}(2a_g + b_g\|\mathbf{u}_g\|_2^2 + 2c_g\mathbf{v}_g^\top\mathbf{u}_g) - \frac{1}{2}\sqrt{\Delta_g},$$

where

$$a_g = \gamma\frac{w_g}{r_g^3}\mathbf{u}_g^\top\mathbf{v}_g + \frac{w_g}{r_g}, \qquad b_g = -\left(\gamma\frac{3w_g}{r_g^5}\mathbf{u}_g^\top\mathbf{v}_g + \frac{w_g}{r_g^3}\right), \qquad c_g = \gamma\frac{w_g}{r_g^3} > 0, \tag{28}$$

and

$$\begin{aligned}
\Delta_g &= 4c_g^2r_g^2\|\mathbf{v}_g\|_2^2 + b_g^2r_g^4 + 4b_gc_gr_g^2\mathbf{u}_g^\top\mathbf{v}_g \\
&= -\frac{3\gamma^2w_g^2}{r_g^6}(\mathbf{u}_g^\top\mathbf{v}_g)^2 + \frac{2\gamma w_g^2}{r_g^4}\mathbf{u}_g^\top\mathbf{v}_g + \frac{4\gamma^2w_g^2\|\mathbf{v}_g\|_2^2}{r_g^4} + \frac{w_g^2}{r_g^2},
\end{aligned} \tag{29}$$

for $g = 1, \ldots, G$. Moreover, $\Delta_g \geq 0$, by Lemma 4 in the Supplementary Materials. Let us now consider the sum and product of the eigenvalues $\lambda_{1,g}$ and $\lambda_{3,g}$. We have:

$$\begin{aligned}
\lambda_{1,g} + \lambda_{3,g} &= 2a_g + b_g\|\mathbf{u}_g\|_2^2 + 2c_g\mathbf{v}_g^\top\mathbf{u}_g \\
&= 2\left(\gamma\frac{w_g}{r_g^3}\mathbf{u}_g^\top\mathbf{v}_g + \frac{w_g}{r_g}\right) - \left(\gamma\frac{3w_g}{r_g^5}\mathbf{u}_g^\top\mathbf{v}_g + \frac{w_g}{r_g^3}\right)r_g^2 + 2\gamma\frac{w_g}{r_g^3}\mathbf{u}_g^\top\mathbf{v}_g \\
&= \frac{\gamma w_g}{r_g^3}\mathbf{u}_g^\top\mathbf{v}_g + \frac{w_g}{r_g} = a_g = \lambda_{2,g},
\end{aligned} \tag{30}$$

therefore $\lambda_{1,g} + \lambda_{3,g} \geq 0$ if $\rho_{u,v} \geq -\frac{r_g}{\gamma\|\mathbf{v}_g\|_2}$, where $\rho_{u,v} = \frac{\mathbf{u}_g^\top\mathbf{v}_g}{\|\mathbf{u}_g\|_2\|\mathbf{v}_g\|_2}$. As concerns the product of $\lambda_{1,g}$ and $\lambda_{3,g}$, we have:

$$\begin{aligned}
\lambda_{1,g}\lambda_{3,g} &= \frac{1}{4}(2a_g + b_g\|\mathbf{u}_g\|_2^2 + 2c_g\mathbf{v}_g^\top\mathbf{u}_g)^2 - \frac{1}{4}\Delta_g \\
&= a_g^2 + \frac{1}{4}b_g^2r_g^4 + c_g^2(\mathbf{u}_g^\top\mathbf{v}_g)^2 + a_gb_gr_g^2 + 2a_gc_g(\mathbf{u}_g^\top\mathbf{v}_g) + b_gc_gr_g^2(\mathbf{u}_g^\top\mathbf{v}_g) \\
&\quad - c_g^2r_g^2\|\mathbf{v}_g\|_2^2 - \frac{1}{4}b_g^2r_g^4 - b_gc_gr_g^2\mathbf{u}_g^\top\mathbf{v}_g \\
&= a_g^2 + a_gb_gr_g^2 - c_g^2\|\mathbf{u}_g\|_2^2\|\mathbf{v}_g\|_2^2(1 - \rho_{u,v}^2) + 2a_gc_g\mathbf{u}_g^\top\mathbf{v}_g.
\end{aligned}$$

Now, we substitute the values of a_g, b_g and c_g in Equation (28) and we get:

$$\lambda_{1,g}\lambda_{3,g} = \left(\gamma\frac{w_g}{r_g^3}\mathbf{u}_g^\top\mathbf{v}_g + \frac{w_g}{r_g}\right)^2 - \left(\gamma\frac{w_g}{r_g^3}\mathbf{u}_g^\top\mathbf{v}_g + \frac{w_g}{r_g}\right)\left(\gamma\frac{3w_g}{r_g^5}\mathbf{u}_g^\top\mathbf{v}_g + \frac{w_g}{r_g^3}\right)r_g^2$$

$$- \gamma^2\frac{w_g^2}{r_g^6}r_g^2\|\mathbf{v}_g\|_2^2(1 - \rho_{u,v}^2) + 2\left(\gamma\frac{w_g}{r_g^3}\mathbf{u}_g^\top\mathbf{v}_g + \frac{w_g}{r_g}\right)\gamma\frac{w_g}{r_g^3}\mathbf{u}_g^\top\mathbf{v}_g$$

$$= \frac{\gamma^2 w_g^2}{r_g^6}\|\mathbf{u}_g\|_2^2\|\mathbf{v}_g\|_2^2(\rho_{u,v}^2 - 1).$$

Therefore, $\lambda_{1,g}\lambda_{3,g} < 0$ and the matrix $\boldsymbol{\Pi}_{\mathcal{A}_G} + \gamma\mathrm{d}\boldsymbol{\Pi}_{\mathcal{A}_G}/\mathrm{d}\gamma$ is indefinite, unless $\rho_{u,v} = 1$ (e.g. $\mathbf{u}_g \propto \mathbf{v}_g$) when it is equal to $\lambda_{1,g}\lambda_{3,g} = 0$. In particular, when $\mathbf{X}^\top\mathbf{X} = \mathbf{I}_p$ then $\rho_{u,v} = 1$ (see Corollary S.5 in Supplementary Materials) and $\lambda_{3,g} = \frac{1}{2}(2a_g + b_g r_g^2 + 2cv\mathbf{u}_g^\top\mathbf{v}_g) - \frac{1}{2}\sqrt{\Delta_g}$ where Δ_g is defined in Equation (29) as:

$$\Delta_{g,\mathrm{ortho}} = -\frac{3\gamma^2 w_g^2}{r_g^6}\rho_{u,v}^2 r_g^2\|\mathbf{v}_g\|_2^2 + \frac{2\gamma w_g^2}{r_g^4}\rho_{u,v}r_g\|\mathbf{v}_g\|_2 + \frac{4\gamma^2 w_g^2\|\mathbf{v}_g\|_2^2}{r_g^4} + \frac{w_g^2}{r_g^2}$$

$$= \frac{\gamma^2 w_g^2\|\mathbf{v}_g\|_2^2}{r_g^4} + \frac{2\gamma w_g^2\|\mathbf{v}_g\|_2}{r_g^3} + \frac{w_g^2}{r_g^2} = \left(\frac{\gamma w_g\|\mathbf{v}_g\|_2}{r_g^2} + \frac{w_g}{r_g}\right)^2 = a_g^2.$$

Moreover, by Equation (30), the first part of $\lambda_{3,g}$, $2a_g + b_g r_g^2 + 2c_g\mathbf{u}_g^\top\mathbf{v}_g = a_g$, therefore $\lambda_{3,g} = a - \sqrt{a^2} = 0$ and $\lambda_{1,g} = \lambda_{2,g}$. Also, $\mathbf{u}_g^\top\mathbf{v}_g = \|\mathbf{u}_g\|_2\|\mathbf{v}_g\|_2$ and a_g defined in Equation (28) is strictly positive, and the matrix $\boldsymbol{\Pi}_g + \gamma\mathrm{d}\boldsymbol{\Pi}_g/\mathrm{d}\gamma$ is positive semidefinite. To check if the orthonormal design is the only setting leading to $\rho_{u,v} = 1$, we observe that $\rho_{u,v} = 1$ implies $\mathbf{R}_{\mathcal{A}_G}^\star\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G} = c\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}$, which in turn means that $\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}$ is an eigenvector of the matrix $\mathbf{R}_{\mathcal{A}_G}^* = \mathbf{R}_{\mathcal{A}_G}\mathbf{W}_{\mathcal{A}_G} = (\mathbf{X}_{\mathcal{A}_G}^\top\mathbf{X}_{\mathcal{A}_G} + \gamma\boldsymbol{\Pi}_{\mathcal{A}_G})^{-1}\mathbf{W}_{\mathcal{A}_G}$, which completes the proof. $\square$

Proof of Theorem 6. The first order conditions for the problem in Equation (13) are represented by

$$-\mathbf{X}_{\mathcal{A}_G}^\top\left(\mathbf{y} - \mathbf{X}_{\mathcal{A}_G}\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}\right) + \gamma\mathbf{W}_{\mathcal{A}_G}\breve{\boldsymbol{\beta}}_{\mathcal{A}_G} = \mathbf{0}$$

where $\mathbf{X}_{\mathcal{A}_G}$, $\mathbf{W}_{\mathcal{A}_G}$ and $\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}$ are restricted to the active set $\mathcal{A}_G$, and $\breve{\boldsymbol{\beta}}_{\mathcal{A}_G} = (\widehat{\boldsymbol{\beta}}_1/\|\widehat{\boldsymbol{\beta}}_1\|_2, \ldots, \widehat{\boldsymbol{\beta}}_G/\|\widehat{\boldsymbol{\beta}}_G\|_2)$. Similarly to Lasso and Adaptive Lasso, by manipulating terms, focusing on the orthonormal design, we arrive to

$$\widehat{\boldsymbol{\beta}}_{\mathcal{A}_G} = (\mathbf{X}_{\mathcal{A}_G}^\top\mathbf{X}_{\mathcal{A}_G})^{-1}(\mathbf{X}_{\mathcal{A}_G}^\top\mathbf{y} - \gamma\mathbf{W}_{\mathcal{A}_G}\breve{\boldsymbol{\beta}}_{\mathcal{A}_G}) = \mathbf{X}_{\mathcal{A}_G}^\top\mathbf{y} - \gamma\mathbf{W}_{\mathcal{A}_G}\breve{\boldsymbol{\beta}}_{\mathcal{A}_G},$$

and if we denote

$$\mathbf{H}_\gamma(\mathbf{y}) = \mathbf{X}_{\mathcal{A}_G}\mathbf{X}_{\mathcal{A}_G}^\top, \qquad \eta_\gamma(\mathbf{y}) = \mathbf{X}_{\mathcal{A}_G}\mathbf{W}_{\mathcal{A}_G}\breve{\boldsymbol{\beta}}_{\mathcal{A}_G},$$

we can also derive the equation linking $\widehat{\mathbf{y}}_\gamma$ and $\mathbf{y}$

$$\widehat{\mathbf{y}}_\gamma = \mathbf{X}\widehat{\boldsymbol{\beta}} = \mathbf{H}_\gamma(\mathbf{y})\mathbf{y} - \gamma\eta_\gamma(\mathbf{y}).$$

The general approach is to start again from Equation (18), and derive an expression similar to Equation (19). However, in Adaptive Group Lasso we see that both $\mathbf{W}_{\mathcal{A}_G}$ —like Adaptive Lasso— and $\breve{\boldsymbol{\beta}}_{\mathcal{A}_G}$ —like Group Lasso— are not constant with respect to $\mathbf{y}$, thus a slight different approach should be employed to find the gradient of $\eta_\gamma(\mathbf{y})$. In particular we make use of the product rule for differentiation in the following way. Let $\eta_0 = \mathbf{X}_{\mathcal{A}_G}(\mathbf{X}_{\mathcal{A}_G}^\top\mathbf{X}_{\mathcal{A}_G})^{-1}$, $\eta_1(\mathbf{y}) = \mathbf{W}_{\mathcal{A}_G}(\mathbf{y})$ and $\eta_2(\mathbf{y}) = \breve{\boldsymbol{\beta}}_{\mathcal{A}_G}(\mathbf{y})$ and rewrite $\eta(\mathbf{y}) = \eta_0\eta_1(\mathbf{y})\eta_2(\mathbf{y})$. Then,

$$\frac{\partial\eta_\gamma(\mathbf{y})}{\partial\mathbf{y}} = \eta_0\left\{\left[\frac{\partial\eta_1(\mathbf{y})}{\partial\mathbf{y}}\right]\eta_2(\mathbf{y}) + \eta_1(\mathbf{y})\frac{\partial\eta_2(\mathbf{y})}{\partial\mathbf{y}}\right\},$$

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where the former multiplication represents a tensor–vector contraction on the second axis, and the latter a standard matrix multiplication. By proceeding with similar arguments to those in the proof of Theorem 2 we have

$$\frac{\partial \widehat{\mathbf{y}}_\gamma}{\partial \mathbf{y}} = \mathbf{H}_\gamma(\mathbf{y}) - \gamma \frac{\partial \eta_\gamma(\mathbf{y})}{\partial \mathbf{y}} = \mathbf{H}_\gamma(\mathbf{y}) - \gamma \eta_0 \left\{ \left[\frac{\partial \eta_1(\mathbf{y})}{\partial \mathbf{y}} \right] \eta_2(\mathbf{y}) + \eta_1(\mathbf{y}) \frac{\partial \eta_2(\mathbf{y})}{\partial \mathbf{y}} \right\},$$

$$= \mathbf{H}_\gamma(\mathbf{y}) - \gamma \eta_0 \left[\frac{\partial \eta_1(\mathbf{y})}{\partial \mathbf{y}} \right] \eta_2(\mathbf{y}) - \gamma \eta_0 \eta_1(\mathbf{y}) \frac{\partial \eta_2(\mathbf{y})}{\partial \mathbf{y}},$$

$$= \mathbf{H}_\gamma(\mathbf{y}) - \gamma \eta_0 \left[\frac{\partial \eta_1(\mathbf{y})}{\partial \mathbf{y}} \right] \eta_2(\mathbf{y}) - \gamma \eta_0 \eta_1(\mathbf{y}) \frac{\partial \eta_2(\mathbf{y})}{\partial \widehat{\mathbf{y}}} \frac{\partial \widehat{\mathbf{y}}_\gamma}{\partial \mathbf{y}},$$

and, by isolating the quantity of interest, we obtain

$$\frac{\partial \widehat{\mathbf{y}}_\gamma}{\partial \mathbf{y}} = \left(\mathbf{I}_n + \gamma \eta_0 \eta_1(\mathbf{y}) \frac{\partial \eta_2(\mathbf{y})}{\partial \widehat{\mathbf{y}}} \right)^{-1} \left(\mathbf{H}_\gamma(\mathbf{y}) - \gamma \eta_0 \left[\frac{\partial \eta_1(\mathbf{y})}{\partial \mathbf{y}} \right] \eta_2(\mathbf{y}) \right). \tag{31}$$

The computation of $\partial \eta_2(\mathbf{y})/\partial \widehat{\mathbf{y}}$ is analogous to that in the proof of Theorem 2. In order to compute the new part we observe that $\mathbf{W}_{\mathcal{A}_G}$ is diagonal and relevant simplifications apply. Specifically, we have

$$\left[\frac{\partial \eta_1(\mathbf{y})}{\partial \mathbf{y}} \right] \eta_2(\mathbf{y}) = \operatorname{diag}(\breve{\boldsymbol{\beta}}_{\mathcal{A}_G}) \frac{\partial \mathbf{W}_{\mathcal{A}_G}(\mathbf{y})}{\partial \mathbf{y}} = \sum_{g \in \mathcal{A}_G} \breve{\beta}_g \frac{\partial w_g(\mathbf{y})}{\partial \mathbf{y}}.$$

The last step is to manipulate the gradient of weights through the chain rule, recalling the assumption $w_g(\mathbf{y}) = w_g(\|\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}}\|_2)$.

$$\frac{\partial w_g(\mathbf{y})}{\partial \mathbf{y}} = \frac{\partial w_g(\|\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}}\|_2)}{\partial \mathbf{y}} = \frac{\partial w_g(\|\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}}\|_2)}{\partial \|\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}}\|_2} \frac{\partial \|\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}}\|_2}{(\partial \widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}})^\top} \frac{\partial (\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}})^\top}{\partial \mathbf{y}} = \frac{\partial w_g(\|\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}}\|_2)}{\partial \|\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}}\|_2} \frac{(\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}})^\top}{\|\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}}\|_2} \mathbf{X}_g^\top,$$

thus

$$\eta_0 \left[\frac{\partial \eta_1(\mathbf{y})}{\partial \mathbf{y}} \right] \eta_2(\mathbf{y}) = \mathbf{X}_{\mathcal{A}_G} \boldsymbol{\Phi}_{\mathcal{A}_G} \mathbf{X}_{\mathcal{A}_G}^\top,$$

where

$$\boldsymbol{\Phi}_{\mathcal{A}_G} = \operatorname{blockdiag}\left(\frac{\widehat{\boldsymbol{\beta}}_g}{\|\widehat{\boldsymbol{\beta}}_g\|_2} \frac{\partial w_g(\|\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}}\|_2)}{\partial \|\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}}\|_2} \frac{(\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}})^\top}{\|\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}}\|_2} \right)$$

To compute degrees of freedom, from Equation (31) we write

$$\widehat{df}_\gamma = \operatorname{trace}\left(\frac{\partial \widehat{\mathbf{y}}_\gamma}{\partial \mathbf{y}} \right) = \operatorname{trace}\left[\left(\mathbf{I}_n + \gamma \eta_0 \eta_1(\mathbf{y}) \frac{\partial \eta_2(\mathbf{y})}{\partial \widehat{\mathbf{y}}} \right)^{-1} \left(\mathbf{H}_\gamma(\mathbf{y}) - \gamma \eta_0 \left[\frac{\partial \eta_1(\mathbf{y})}{\partial \mathbf{y}} \right] \eta_2(\mathbf{y}) \right) \right]$$

$$= \operatorname{trace}\left[\left(\mathbf{I}_n + \gamma \mathbf{X}_{\mathcal{A}_G} \boldsymbol{\Pi}_{\mathcal{A}_G} \mathbf{X}_{\mathcal{A}_G}^\top \right)^{-1} \left(\mathbf{X}_{\mathcal{A}_G} \mathbf{X}_{\mathcal{A}_G}^\top - \gamma \mathbf{X}_{\mathcal{A}_G} \boldsymbol{\Phi}_{\mathcal{A}_g} \mathbf{X}_{\mathcal{A}_G}^\top \right) \right],$$

completing the proof for the orthonormal case. For non-orthonormal designs we have $\mathbf{H}_\gamma(\mathbf{y}) = \mathbf{X}_{\mathcal{A}_G}(\mathbf{X}_{\mathcal{A}_G}^\top \mathbf{X}_{\mathcal{A}_G})^{-1}\mathbf{X}_{\mathcal{A}_G}^\top$ and $\eta_\gamma(\mathbf{y}) = \mathbf{X}_{\mathcal{A}_G}(\mathbf{X}_{\mathcal{A}_G}^\top \mathbf{X}_{\mathcal{A}_G})^{-1}\mathbf{W}_{\mathcal{A}_G}\breve{\boldsymbol{\beta}}_{\mathcal{A}_G}$. Previous computations can be done in a similar manner by considering $\eta_0 = \mathbf{X}_{\mathcal{A}_G}(\mathbf{X}_{\mathcal{A}_G}^\top \mathbf{X}_{\mathcal{A}_G})^{-1}$, directly leading to the result. $\square$

Proof of Corollary 6. Under the setting of Theorem 6 and the orthonormal design assumption, we have that and $\widehat{\boldsymbol{\beta}}^{\mathsf{LS}} = \mathbf{X}^\top \mathbf{y}$ and the generic term of the matrix $\mathbf{W}$ is given by $w_{gg} =$

$w_g(\|\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}}\|_2) = 1/\|\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}}\|_2 = 1/\|\mathbf{X}_g^\top \mathbf{y}\|_2$. By applying the result of Theorem 6 in the orthonormal case we have

$$\left.\frac{\partial w_g(z)}{\partial z}\right|_{z=\widehat{\beta}_g^{\mathsf{LS}}} = \left.\frac{\partial}{\partial z}\left(\frac{1}{z}\right)\right|_{z=\widehat{\beta}_g^{\mathsf{LS}}} = \left.-\frac{1}{z^2}\right|_{z=\widehat{\beta}_g^{\mathsf{LS}}} = -\frac{1}{\|\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}}\|_2^2},$$

which concludes the proof. $\square$

Proof of Corollary 7. Under the setting of Theorem 6, we have $\widehat{\boldsymbol{\beta}}^{\mathsf{LS}} = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}$ and the generic term of the matrix $\mathbf{W}$ is given by $w_{gg} = w_g(\|\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}}\|_2) = 1/\|\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}}\|_2 = 1/\|\mathbf{p}_g^\top \mathbf{y}\|_2$, where $\mathbf{p}_g \in \mathbb{R}^n$ is the matrix $\mathbf{P} = \mathbf{X}(\mathbf{X}^\top\mathbf{X})^{-1} \in \mathbb{R}^{n\times p}$ restricted to the g-th group. By applying the result of Theorem 6 in the non-orthonormal case we have

$$\left.\frac{\partial w_g(z)}{\partial z}\right|_{z=\widehat{\beta}_g^{\mathsf{LS}}} = \left.\frac{\partial}{\partial z}\left(\frac{1}{z}\right)\right|_{z=\widehat{\beta}_g^{\mathsf{LS}}} = \left.-\frac{1}{z^2}\right|_{z=\widehat{\beta}_g^{\mathsf{LS}}} = -\frac{1}{\|\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}}\|_2^2},$$

which concludes the proof. $\square$

Proof of Corollary 8. We show that

$$\begin{aligned}
\mathrm{trace}\big[(\mathbf{I}_p + \gamma\mathbf{B})^{-1}\mathbf{A}\big] &\leq \mathrm{trace}\big[(\mathbf{I}_p + \gamma\mathbf{B})^{-1}(\mathbf{A} - \gamma\mathbf{C})\big]\\
&= \mathrm{trace}\big[(\mathbf{I}_p + \gamma\mathbf{B})^{-1}\mathbf{A}\big] - \gamma\,\mathrm{trace}\big[(\mathbf{I}_p + \gamma\mathbf{B})^{-1}\mathbf{C}\big].
\end{aligned}$$

Since $\gamma > 0$, $\mathbf{I}_p$ and $\mathbf{B}$ are positive definite, the previous inequality is true if $\mathbf{C}$ is negative semidefinite, and thus if the quantity

$$\boldsymbol{\Phi}_{\mathcal{A}_G} = \mathrm{blockdiag}\left(\frac{\widehat{\boldsymbol{\beta}}_g}{\|\widehat{\boldsymbol{\beta}}_g\|_2}\frac{\partial w_g(\|\widehat{\boldsymbol{\beta}}^{\mathsf{LS}}\|_2)}{\partial\|\widehat{\boldsymbol{\beta}}^{\mathsf{LS}}\|_2}\frac{(\widehat{\boldsymbol{\beta}}^{\mathsf{LS}})^\top}{\|\widehat{\boldsymbol{\beta}}^{\mathsf{LS}}\|_2}\right),$$

is negative semidefinite. By examination of this matrix, we conclude that both $\|\widehat{\boldsymbol{\beta}}_g\|_2$ and $\|\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}}\|_2$ are positive, $\partial w_g(\|\widehat{\boldsymbol{\beta}}^{\mathsf{LS}}\|_2)/\partial\|\widehat{\boldsymbol{\beta}}^{\mathsf{LS}}\|_2$ is a negative scalar by assumption and the matrix $\widehat{\boldsymbol{\beta}}_g(\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}})^\top$ is positive semidefinite only if $(\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}})^\top\widehat{\boldsymbol{\beta}}_g \geq 0$. $\square$

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Supplementary materials for:
On the Degrees of Freedom of some Lasso procedures

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These supplementary materials are organized as follows. Section S.1 provides additional results together with their proofs, and Section S.2 collects several technical lemmas and auxiliary results used throughout the paper.

S.1 Additional results

Corollary S.1. *Let* $\mathbf{X}^\top\mathbf{X} = \mathbf{I}_p$, $\widehat{\boldsymbol{\beta}}$ *the solution to the Adaptive Lasso problem in Equation* (4) *with weights equal to* $w_j = \exp(-\alpha|\widehat{\beta}_j^{\mathsf{LS}}|)$ *and* $\gamma \in (\gamma_l, \gamma_{l+1})$. *Denote with* $\mathcal{A}$ *the corresponding active set. An unbiased estimate of the degrees of freedom is*

$$\widehat{df}_\gamma = |\mathcal{A}| + \gamma \sum_{j \in \mathcal{A}} \frac{\alpha}{\exp(\alpha|\widehat{\beta}_j^{\mathsf{LS}}|)}.$$

Proof. Under the setting of Theorem 1 and the orthonormal design assumption, we have that $\mathbf{H}_\gamma(\mathbf{y}) = \mathbf{X}_\mathcal{A}\mathbf{X}_\mathcal{A}^\top$, $\eta_\gamma(\mathbf{y}) = \mathbf{X}_\mathcal{A}\mathbf{W}_\mathcal{A}(\mathbf{y})\mathrm{sgn}(\widehat{\boldsymbol{\beta}}_\mathcal{A})$ and $\widehat{\boldsymbol{\beta}}^{\mathsf{LS}} = \mathbf{X}^\top\mathbf{y}$. Moreover, the matrix $\mathbf{W}$ is given by

$$\mathbf{W} = \mathrm{diag}\Big(\frac{1}{\exp(\alpha|\widehat{\boldsymbol{\beta}}^{\mathsf{LS}}|)}\Big) = \mathrm{diag}\Big(\frac{1}{\exp(\alpha|\mathbf{X}^\top\mathbf{y}|)}\Big),$$

with generic term being $w_{jj} = w_j(|\widehat{\beta}_j^{\mathsf{LS}}|) = 1/\exp(\alpha|\widehat{\beta}_j^{\mathsf{LS}}|) = 1/\exp(\alpha|\mathbf{x}_j^\top\mathbf{y}|)$. By applying the result of Theorem 1 in the orthonormal case we have

$$\frac{\partial w_j(z)}{\partial z}\Big|_{z=\widehat{\beta}_j^{\mathsf{LS}}} = \frac{\partial}{\partial z}\Big(\frac{1}{\exp(\alpha z)}\Big)\Big|_{z=\widehat{\beta}_j^{\mathsf{LS}}} = -\frac{\alpha}{\exp(\alpha z)}\Big|_{z=\widehat{\beta}_j^{\mathsf{LS}}} = -\frac{\alpha}{\exp(\alpha|\widehat{\beta}_j^{\mathsf{LS}}|)},$$

which concludes the proof. $\square$

Corollary S.2. *Let* $\widehat{\boldsymbol{\beta}}$ *be the solution to the Adaptive Lasso problem in Equation* (4) *with weights equal to* $w_j = \exp(-\alpha|\widehat{\beta}_j^{\mathsf{LS}}|)$ *and* $\gamma \in (\gamma_l, \gamma_{l+1})$. *Denote with* $\mathcal{A}$ *the corresponding active set. An unbiased estimate of the degrees of freedom is*

$$\widehat{df}_\gamma = |\mathcal{A}| + \gamma\alpha \sum_{j \in \mathcal{A}} \mathrm{sgn}(\widehat{\beta}_j)\frac{\mathrm{sgn}(\widehat{\beta}_j^{\mathsf{LS}})}{\exp(\alpha|\widehat{\beta}_j^{\mathsf{LS}}|)}[(\mathbf{X}_\mathcal{A}^\top\mathbf{X}_\mathcal{A})^{-1}]_{\pi(j),\pi(j)}.$$

Proof. Under the setting of Theorem 1, we have $\widehat{\boldsymbol{\beta}}^{\mathsf{LS}} = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}$ and

$$\mathbf{W} = \mathrm{diag}\Big(\frac{1}{\exp(\alpha|\widehat{\boldsymbol{\beta}}^{\mathsf{LS}}|)}\Big) = \mathrm{diag}\Big(\frac{1}{\exp(\alpha|(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}|)}\Big),$$

with generic term being $w_{jj} = w_j(|\widehat{\beta}_j^{\mathsf{LS}}|) = 1/\exp(\alpha|\widehat{\beta}_j^{\mathsf{LS}}|) = 1/\exp(\alpha|\mathbf{p}_j^\top\mathbf{y}|)$, where $\mathbf{p}_j \in \mathbb{R}^n$ is the j-th column of $\mathbf{P} = \mathbf{X}(\mathbf{X}^\top\mathbf{X})^{-1} \in \mathbb{R}^{n \times p}$. By applying the result of Theorem 1 in the

non-orthonormal case we have

$$\left.\frac{\partial w_j(z)}{\partial z}\right|_{z=\widehat{\beta}_j^{\mathsf{LS}}} = \left.\frac{\partial}{\partial z}\left(\frac{1}{\exp(\alpha z)}\right)\right|_{z=\widehat{\beta}_j^{\mathsf{LS}}} = \left.-\frac{\alpha}{\exp(\alpha z)}\right|_{z=\widehat{\beta}_j^{\mathsf{LS}}} = -\frac{\alpha}{\exp(\alpha|\widehat{\beta}_j^{\mathsf{LS}}|)},$$

which concludes the proof. $\square$

Corollary S.3. *Under the settings of Theorem 2, the following are equivalent*

$$\widehat{df}_\gamma = |\mathcal{A}_G| + \sum_{g\in\mathcal{A}_G} \frac{n_g - 1}{1 + \gamma\frac{w_g}{\|\boldsymbol{\beta}_g\|_2}}$$

$$\widehat{df}_\gamma = |\mathcal{A}_p| - \sum_{g\in\mathcal{A}_G} (n_g - 1)\frac{\gamma w_g/\|\boldsymbol{\beta}_g\|_2}{1 + \gamma w_g/\|\boldsymbol{\beta}_g\|_2}.$$

Proof. The eigenvalues of $\mathbf{A}$ and $\mathbf{B}$ are, respectively,

$$\lambda(\mathbf{A}) = (\underbrace{1,\ldots,1}_{|\mathcal{A}_p|}, \underbrace{0,\ldots,0}_{n-|\mathcal{A}_p|}), \quad \lambda(\mathbf{B}) = \left(\bigcup_{g\in\mathcal{A}}\left\{\underbrace{\frac{w_g}{\|\widehat{\boldsymbol{\beta}}_g\|_2},\ldots,\frac{w_g}{\|\widehat{\boldsymbol{\beta}}_g\|_2},0}_{n_g-1}\right\}, \underbrace{0,\ldots,0}_{n-|\mathcal{A}_p|}\right),$$

thus $\mathbf{B}$ has $|\mathcal{A}_p| - |\mathcal{A}_G|$ eigenvalues greater than zero. We have that

$$\operatorname{trace}((\mathbf{I}_n + \gamma\mathbf{B})^{-1}\mathbf{A}) = \sum_{i=1}^n \frac{\lambda_i^A}{1 + \gamma\lambda_i^B} = \sum_{g\in\mathcal{A}_G}\sum_{j=1}^{n_g} \frac{\lambda_{n_{g-1}+j}^A}{1 + \gamma\lambda_{n_{g-1}+j}^B} = \sum_{g\in\mathcal{A}_G}\left\{\sum_{j=1}^{n_g-1}\frac{1}{1+\gamma\frac{w_g}{\|\widehat{\boldsymbol{\beta}}_g\|_2}} + 1\right\}$$

$$= |\mathcal{A}_G| + \sum_{g\in\mathcal{A}_G}\sum_{j=1}^{n_g-1}\frac{1}{1+\gamma\frac{w_g}{\|\widehat{\boldsymbol{\beta}}_g\|_2}} = |\mathcal{A}_G| + \sum_{g\in\mathcal{A}_G}\frac{n_g-1}{1+\gamma\frac{w_g}{\|\widehat{\boldsymbol{\beta}}_g\|_2}},$$

which is the result presented in Yuan and Lin (2006). By contrast,

$$\operatorname{trace}((\mathbf{I}_n + \gamma\mathbf{B})^{-1}\mathbf{A}) = \operatorname{trace}(\mathbf{A} - \gamma\mathbf{B}(\mathbf{I}_n + \gamma\mathbf{B})^{-1}\mathbf{A})$$

$$= \operatorname{trace}(\mathbf{A}) - \operatorname{trace}(\gamma\mathbf{B}(\mathbf{I}_n + \gamma\mathbf{B})^{-1}\mathbf{A})$$

$$= |\mathcal{A}_p| - \sum_{i=1}^n \frac{\gamma\lambda_i^B}{1+\gamma\lambda_i^B}\lambda_i^A = |\mathcal{A}_p| - \sum_{g\in\mathcal{A}_G}\sum_{j=1}^{n_g}\frac{\gamma\lambda_{n_{g-1}+j}^B}{1+\gamma\lambda_{n_{g-1}+j}^B}\lambda_{n_{g-1}+j}^A$$

$$= |\mathcal{A}_p| - \sum_{g\in\mathcal{A}_G}\sum_{j=1}^{n_g-1}\frac{\gamma w_g/\|\widehat{\boldsymbol{\beta}}_g\|_2}{1+\gamma w_g/\|\widehat{\boldsymbol{\beta}}_g\|_2} = |\mathcal{A}_p| - \sum_{g\in\mathcal{A}_G}(n_g-1)\frac{\gamma w_g/\|\widehat{\boldsymbol{\beta}}_g\|_2}{1+\gamma w_g/\|\widehat{\boldsymbol{\beta}}_g\|_2},$$

which is the result presented in Vaiter et al. (2017). Similar simplifications under the non orthonormal setting are not easy to derive, as this proof is based on the eigenvalues of the matrix $\mathbf{B}$ which are unknown unless $\mathbf{X}^\top\mathbf{X} = \mathbf{I}_p$. $\square$

Corollary S.4. *Under the settings of Theorems 2 and 3, if $n_g = 1$ for all $g \in \mathcal{G}_G$ we have $\widehat{df} = |\mathcal{A}|$, recovering the Lasso result.*

Proof. In such circumstances the problem in Equation (9) is equivalent to the problem in Equation (4) with fixed weights, $G = p$, $\|\boldsymbol{\beta}_g\|_2 = |\beta_g|$ and $|\mathcal{A}_G| = |\mathcal{A}_p|$. If $\mathbf{X}^\top\mathbf{X} = \mathbf{I}_p$, starting from Corollary 3 we have that $n_g = 1$, and the result is $\widehat{df} = |\mathcal{A}|$, which is the number of active groups and active variables at the same time. For the non-orthogonal case, it turns out that $\|\boldsymbol{\beta}_g\|_2^2 = \boldsymbol{\beta}_g^\top\boldsymbol{\beta}_g = \boldsymbol{\beta}_g\boldsymbol{\beta}_g^\top$ and $\boldsymbol{\Pi}_\mathcal{A}$ is null, and we have again that $\widehat{df} = \operatorname{trace}(\mathbf{A}) = \operatorname{trace}(\mathbf{H}_\gamma) = |\mathcal{A}|$. $\square$

Corollary S.5. *Under the setting of Theorem [4], for the orthonormal design, $\mathbf{X}^\top \mathbf{X} = \mathbf{I}_p$, we have:*

$$\frac{\mathrm{d}\widehat{\boldsymbol{\beta}}_g}{\mathrm{d}\gamma} = -\frac{w_g}{r_g}\widehat{\boldsymbol{\beta}}_g, \qquad \frac{\mathrm{d}r_g}{\mathrm{d}\gamma} = -w_g, \qquad \frac{\mathrm{d}\boldsymbol{\Pi}_g}{\mathrm{d}\gamma} = \frac{w_g}{r_g}\boldsymbol{\Pi}_g, \qquad \text{for each } g \in \mathcal{A}_G,$$

where $r_g = \|\widehat{\boldsymbol{\beta}}_g\|_2$, which means that the solution scales linearly in the direction of $\widehat{\boldsymbol{\beta}}_g$ as γ increases, for each active group.

Proof. Let us compute the expression for the derivative of $\widehat{\boldsymbol{\beta}}_g$ with respect to the regularization parameter γ, when $\mathbf{X}^\top \mathbf{X} = \mathbf{I}_p$. Equation (25) reduces to the following expression:

$$\frac{\mathrm{d}\widehat{\boldsymbol{\beta}}_g}{\mathrm{d}\gamma} = -\frac{w_g}{r_g}(\mathbf{I}_{n_g} + \gamma \boldsymbol{\Pi}_g)^{-1}\widehat{\boldsymbol{\beta}}_g, \tag{S.1}$$

where $r_g = \|\widehat{\boldsymbol{\beta}}_g\|_2$ and $\boldsymbol{\Pi}_g$ has been defined in Equation (11). Since $\boldsymbol{\Pi}_g$ is symmetric, it can be diagonalized. Consider the eigensystem of $\boldsymbol{\Pi}_g$. The direction $\widehat{\boldsymbol{\beta}}_g$ is an eigenvector of $\boldsymbol{\Pi}_g$. Let $\mathbf{u}_g = \widehat{\boldsymbol{\beta}}_g / \|\widehat{\boldsymbol{\beta}}_g\|_2 = \widehat{\boldsymbol{\beta}}_g / r_g$ be a unit vector, then:

$$\boldsymbol{\Pi}_g \mathbf{u}_g = w_g \left(\frac{\mathbf{I}_{n_g}}{r_g} - \frac{\widehat{\boldsymbol{\beta}}_g \widehat{\boldsymbol{\beta}}_g^\top}{r_g^3}\right)\mathbf{u}_g = w_g \frac{\mathbf{u}_g}{r_g} - w_g \frac{\widehat{\boldsymbol{\beta}}_g \widehat{\boldsymbol{\beta}}_g^\top \mathbf{u}_g}{r_g^3}$$

$$= w_g \frac{\mathbf{u}_g}{r_g} - w_g \frac{\widehat{\boldsymbol{\beta}}_g (\widehat{\boldsymbol{\beta}}_g^\top \mathbf{u}_g)}{r_g^3} = w_g \frac{\mathbf{u}_g}{r_g} - w_g \frac{\widehat{\boldsymbol{\beta}}_g r_g}{r_g^3} = w_g \frac{\mathbf{u}_g}{r_g} - w_g \frac{r_g^2 \mathbf{u}_g}{r_g^3} = 0,$$

therefore, $\mathbf{u}_g$ is an eigenvector with eigenvalue equal to 0. Moreover, for any vector $\mathbf{v}_g \perp \mathbf{u}_g$, we have:

$$\boldsymbol{\Pi}\mathbf{v}_g = w_g \left(\frac{\mathbf{I}_{n_g}}{r_g} - \frac{\widehat{\boldsymbol{\beta}}_g \widehat{\boldsymbol{\beta}}_g^\top}{r_g^3}\right)\mathbf{v}_g = w_g \frac{\mathbf{v}_g}{r} - w_g \frac{\widehat{\boldsymbol{\beta}}_g (\widehat{\boldsymbol{\beta}}_g^\top \mathbf{v}_g)}{r_g^3} = \frac{\mathbf{v}_g}{r_g},$$

so every orthogonal direction to $\widehat{\boldsymbol{\beta}}_g$ has eigenvalue equal to w_g/r_g. Thus, the eigenvalues of $\boldsymbol{\Pi}_g$ are $\lambda_1 = 0$ with multiplicity equal to one, and $\lambda_{n_g} = w_g/r_g$ with multiplicity equal to $n_g - 1$. Therefore, along $\widehat{\boldsymbol{\beta}}_g$ the eigenvalue of $\mathbf{I}_{n_g} + \gamma \boldsymbol{\Pi}_g$ is 1, while orthogonal to $\widehat{\boldsymbol{\beta}}_g$ the eigenvalues of $\mathbf{I}_{n_g} + \gamma \boldsymbol{\Pi}_g$ are $1 + \gamma w_g/r_g$. Let us now compute $\mathrm{d}\widehat{\boldsymbol{\beta}}_g/\mathrm{d}\gamma$ in Equation (S.1). Since $\mathbf{I}_{n_g} + \gamma \boldsymbol{\Pi}_g$ acts as identity on $\widehat{\boldsymbol{\beta}}_g$, the same is true for its inverse, i.e. $(\mathbf{I}_{n_g} + \gamma \boldsymbol{\Pi}_g)^{-1}\widehat{\boldsymbol{\beta}}_g = \widehat{\boldsymbol{\beta}}_g$, and thus

$$\frac{\mathrm{d}\widehat{\boldsymbol{\beta}}_g}{\mathrm{d}\gamma} = -w_g \frac{\widehat{\boldsymbol{\beta}}_g}{r_g},$$

which completes the first part of the proof. Equation (26) in the orthonormal setting reduces to

$$\frac{\mathrm{d}r_g}{\mathrm{d}\gamma} = \frac{\mathrm{d}}{\mathrm{d}\gamma}\left(\|\widehat{\boldsymbol{\beta}}_g\|_2\right) = -\frac{1}{r_g}\widehat{\boldsymbol{\beta}}_g^\top \left[\mathbf{R}_{\mathcal{A}_G}^\star \widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}\right]_g = -\frac{w_g}{r_g^2}\widehat{\boldsymbol{\beta}}_g^\top (\mathbf{I}_{n_g} + \gamma \boldsymbol{\Pi}_g)^{-1}\widehat{\boldsymbol{\beta}}_g = -\frac{w_g}{r_g^2}\widehat{\boldsymbol{\beta}}_g^\top \widehat{\boldsymbol{\beta}}_g = -w_g$$

which completes the second part of the proof. In order to prove the last expression, let us consider Equation (27) in the orthonormal setting:

$$\frac{\mathrm{d}\boldsymbol{\Pi}_g}{\mathrm{d}\gamma} = -\frac{w_g}{r_g^2}\frac{\mathrm{d}r_g}{\mathrm{d}\gamma}\left(\mathbf{I}_{n_g} - \frac{3}{r_g^2}\widehat{\boldsymbol{\beta}}_g \widehat{\boldsymbol{\beta}}_g^\top\right) + \frac{w_g}{r_g^3}\left(\left[\mathbf{R}_{\mathcal{A}_G}^\star \widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}\right]_g \widehat{\boldsymbol{\beta}}_g^\top + \widehat{\boldsymbol{\beta}}_g \left[\mathbf{R}_{\mathcal{A}_G}^\star \widehat{\boldsymbol{\beta}}_{\mathcal{A}_G}\right]_g^\top\right)$$

$$= \frac{w_g^2}{r_g^2}\left(\mathbf{I}_{n_g} - \frac{3}{r_g^2}\widehat{\boldsymbol{\beta}}_g \widehat{\boldsymbol{\beta}}_g^\top\right) + \frac{w_g^2}{r_g^4}\left(\widehat{\boldsymbol{\beta}}_g \widehat{\boldsymbol{\beta}}_g^\top + \widehat{\boldsymbol{\beta}}_g \widehat{\boldsymbol{\beta}}_g^\top\right)$$

$$= \frac{w_g^2}{r_g^2}\left(\mathbf{I}_{n_g} - \frac{3}{r_g^2}\widehat{\boldsymbol{\beta}}_g \widehat{\boldsymbol{\beta}}_g^\top\right) + 2\frac{w_g^2}{r_g^4}\widehat{\boldsymbol{\beta}}_g \widehat{\boldsymbol{\beta}}_g^\top = \frac{w_g^2}{r_g^2}\left(\mathbf{I}_{n_g} - \frac{1}{r_g^2}\widehat{\boldsymbol{\beta}}_g \widehat{\boldsymbol{\beta}}_g^\top\right) = \frac{w_g}{r_g}\boldsymbol{\Pi}_g.$$

$\square$

3

Corollary S.6. *Under the settings of Corollary 6, the following is equivalent to Equation (15).*

$$\widehat{df}_\gamma = |\mathcal{A}_G| + \sum_{g \in \mathcal{A}_G} \left(n_g - 1 + \frac{\gamma}{\|\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}}\|_2^2} \right) \frac{1}{1 + \gamma \frac{w_g}{\|\widehat{\boldsymbol{\beta}}_g\|_2}}$$

Proof. Starting from Equation (15) we have

$$\widehat{df}_\gamma = \text{trace}\big[(\mathbf{I}_n + \gamma\mathbf{B})^{-1}\mathbf{A}\big] + \gamma\,\text{trace}\big[(\mathbf{I}_n + \gamma\mathbf{B})^{-1}\mathbf{C}\big]$$

About the former quantity, as in Group Lasso, we have

$$\text{trace}\big[(\mathbf{I}_n + \gamma\mathbf{B})^{-1}\mathbf{A}\big] = |\mathcal{A}_G| + \sum_{g \in \mathcal{A}_G} \frac{n_g - 1}{1 + \gamma \frac{w_g}{\|\widehat{\boldsymbol{\beta}}_g\|_2}}.$$

For the latter, note that matrix $\mathbf{C}$ is positive semidefinite and, since for the orthonormal design we have $\widehat{\boldsymbol{\beta}}_g = c\widehat{\boldsymbol{\beta}}^{\mathsf{LS}}$ for certain $c > 0$, its spectrum is

$$\lambda(\mathbf{C}) = \left(\bigcup_{g \in \mathcal{A}} \left\{ \frac{1}{\|\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}}\|_2^2}, \underbrace{0, \ldots, 0}_{n_g - 1} \right\}, \underbrace{0, \ldots, 0}_{n - |\mathcal{A}_p|} \right) = \left(\bigcup_{g \in \mathcal{A}} \left\{ \frac{1}{\|\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}}\|_2^2} \right\}, \underbrace{0, \ldots, 0}_{n - |\mathcal{A}_G|} \right).$$

Thus,

$$\text{trace}\big[(\mathbf{I}_n + \gamma\mathbf{B})^{-1}\mathbf{C}\big] = \sum_{i=1}^{n} \frac{\lambda_i^C}{1 + \lambda_i^B} = \sum_{g \in \mathcal{A}_G} \frac{1/\|\widehat{\boldsymbol{\beta}}_g^{\mathsf{LS}}\|_2^2}{1 + \gamma \frac{w_g}{\|\widehat{\boldsymbol{\beta}}_g\|_2}}.$$

which leads directly to the result. $\qquad\square$

Corollary S.7. *Under the settings of Theorems 6 and 7, we recover the Adaptive Lasso as a limiting case when $n_g = 1$ for all $g \in \mathcal{G}_G$, the Group Lasso if weights $w_g(\mathbf{y}) = w_g$ do not depend on $\mathbf{y}$, and the Lasso if both these conditions are satisfied.*

Proof. When $n_g = 1$ the problem in Equation (13) is equivalent to the problem in Equation (4) with adaptive weights, $G = p$, $\|\boldsymbol{\beta}_g\|_2 = |\beta_g|$ and $|\mathcal{A}_G| = |\mathcal{A}_p|$. It turns out that $\|\boldsymbol{\beta}_g\|_2^2 = \boldsymbol{\beta}_g^\top \boldsymbol{\beta}_g = \boldsymbol{\beta}_g \boldsymbol{\beta}_g^\top$ and $\boldsymbol{\Pi}_\mathcal{A}$ is null. Moreover, $\|\widehat{\boldsymbol{\beta}}_g\|_2 = |\widehat{\boldsymbol{\beta}}_g|_1$ and $\|\widehat{\boldsymbol{\beta}}_g\|_2^3 = |\widehat{\boldsymbol{\beta}}_g|_1^3 = \widehat{\boldsymbol{\beta}}_g^2|\widehat{\boldsymbol{\beta}}_g|_1$ and

$$\boldsymbol{\Phi}_{\mathcal{A}_g} = \boldsymbol{\Phi}_j = \frac{\widehat{\beta}_j^{\mathsf{LS}}\widehat{\beta}_j}{|\widehat{\beta}_j^{\mathsf{LS}}||\widehat{\beta}_j|} \left.\frac{\partial w_j(z)}{\partial z}\right|_{z=\widehat{\beta}_j^{\mathsf{LS}}} = \text{sgn}(\widehat{\beta}_j^{\mathsf{LS}})\text{sgn}(\widehat{\beta}_j) \left.\frac{\partial w_j(z)}{\partial z}\right|_{z=\widehat{\beta}_j^{\mathsf{LS}}},$$

which is exactly the quantity that we introduced in Theorem 1. When the weights do not depend on the response, we have $\partial w_g / \partial \mathbf{y} = 0$ and thus $\boldsymbol{\Phi}_\mathcal{A} = \mathbf{0}$ and $\mathbf{C} = \mathbf{0}$ leading directly to Theorem 2 and 3. Finally, if $n_g = 1$ and the weights are independent from $\mathbf{y}$, both simplifications apply, leading to standard Lasso result. $\qquad\square$

S.2 Technical results

Lemma 1. *Let $\mathbf{A} \in \mathbb{R}^{n \times p}$, $\mathbf{b} \in \mathbb{R}^p$ and $\mathbf{W}_y = \text{diag}(f_\varrho(\mathbf{w}_y)) \in \mathbb{S}^{p \times p}$, where $\mathbf{w}_y = \mathbf{P}^\top \mathbf{y} \in \mathbb{R}^p$, with $\mathbf{P} = \mathbf{X}(\mathbf{X}^\top\mathbf{X})^{-1}$, $\mathbf{X} \in \mathbb{R}^{n \times p}$, $\mathbf{y} \in \mathbb{R}^n$ and $f_\varrho(x) : \mathbb{R} \to \mathbb{R}^+$ is a positive function that applies element-wise and $\varrho \in \mathbb{R}$ is an additional parameter controlling the weighting function, then*

$$\frac{\partial(\mathbf{A}\mathbf{W}_y\mathbf{b})}{\partial \mathbf{y}} = \sum_{g=1}^{p} b_g f_\varrho'(\mathbf{p}_g^\top \mathbf{y})\mathbf{p}_g \mathbf{a}_g^\top,$$

where $f'_\varrho(x) : \mathbb{R} \to \mathbb{R}$ is the first derivative of $f_\varrho(x)$, $w_{y,g}$ denotes the g-th diagonal element of the matrix $\mathbf{W}_y$, $\mathbf{p}_g$ and $\mathbf{a}_g$ denote the g-th column of the matrix $\mathbf{P}$, and $\mathbf{A}$ respectively, and $\mathbf{e}_g$ is the g-th column vector of $\mathbf{I}_p$. If $f(x) = |x|^{-1}$, then $\left.\frac{\partial f_\varrho(x)}{\partial x}\right|_{\mathbf{p}_g^\top \mathbf{y}} = \frac{-\text{sgn}(\mathbf{p}_g^\top \mathbf{y})}{(\mathbf{p}_g^\top \mathbf{y})^2}$, while if $f(x) = \exp\left(-\varrho|x|\right)$ then $\left.\frac{\partial f_\varrho(x)}{\partial x}\right|_{\mathbf{p}_g^\top \mathbf{y}} = -\frac{\varrho\text{sgn}(\mathbf{p}_g^\top \mathbf{y})}{\exp\left(\varrho\mathbf{p}_g^\top \mathbf{y}\right)}$.

Proof. By exploiting the properties of the vectorization operator, as detailed in Magnus and Neudecker (1999), we get:

$$\frac{\partial(\mathbf{A}\mathbf{W}_y\mathbf{b})}{\partial \mathbf{y}} = \frac{\partial\text{vec}(\mathbf{A}\mathbf{W}_y\mathbf{b})}{\partial \mathbf{y}} = (\mathbf{b}^\top \otimes \mathbf{A})\frac{\partial\text{vec}(\mathbf{W}_y)}{\partial \mathbf{y}},$$

where

$$\frac{\partial\text{vec}(\mathbf{W}_y)}{\partial \mathbf{y}} = \begin{bmatrix} \mathbf{e}_1\left(\frac{\partial w_{y,1}}{\partial \mathbf{y}}\right)^\top \\ \mathbf{e}_2\left(\frac{\partial w_{y,2}}{\partial \mathbf{y}}\right)^\top \\ \vdots \\ \mathbf{e}_p\left(\frac{\partial w_{y,p}}{\partial \mathbf{y}}\right)^\top \end{bmatrix} \in \mathbb{R}^{p^2 \times n}, \tag{S.2}$$

and using the chain rule for derivatives of composite functions

$$\frac{\partial w_{y,g}}{\partial \mathbf{y}} = f'(\mathbf{p}_g^\top \mathbf{y})\frac{\partial \mathbf{p}_g^\top \mathbf{y}}{\partial \mathbf{y}} = f'(\mathbf{p}_g^\top \mathbf{y})\mathbf{p}_g \in \mathbb{R}^n, \tag{S.3}$$

for all $g = 1, \ldots, p$. Equations (S.2)-(S.3) further simplify to

$$\frac{\partial(\mathbf{A}\mathbf{W}_y\mathbf{b})}{\partial \mathbf{y}} = \sum_{g=1}^{p} b_g \frac{\partial w_{y,g}}{\partial \mathbf{y}}\mathbf{a}_g^\top = \sum_{g=1}^{p} b_g f'(\mathbf{p}_g^\top \mathbf{y})\mathbf{p}_g\mathbf{a}_g^\top.$$

If $f(x) = |x|^{-1}$, then $f'(x) = -\frac{\text{sgn}(x)}{x^2}$ and $\frac{\partial w_{y,g}}{\partial \mathbf{y}} = \frac{-\text{sgn}(\mathbf{p}_g^\top \mathbf{y})}{(\mathbf{p}_g^\top \mathbf{y})^2}\mathbf{p}_g$. If $f(x) = \exp\left(-\varrho|x|\right)$ then $f'(x) = -\varrho f(x)\text{sgn}(x)$ and $\frac{\partial w_{y,g}}{\partial \mathbf{y}} = -\frac{\varrho\text{sgn}(\mathbf{p}_g^\top \mathbf{y})}{\exp\left(\varrho\mathbf{p}_g^\top \mathbf{y}\right)}\mathbf{p}_g$. This completes the proof. $\square$

Lemma 2. *Let* $\mathbf{A} \in \mathbb{R}^{n \times p}$ *and* $\mathbf{x} \in \mathbb{R}^p$, *such that* $\|\mathbf{A}\mathbf{x}\|_2 \neq 0$, *then*

$$\frac{\partial}{\partial \mathbf{x}}\left(\frac{\mathbf{A}^\top \mathbf{A}\mathbf{x}}{\|\mathbf{A}\mathbf{x}\|_2}\right) = \frac{\mathbf{A}^\top \mathbf{A}}{\|\mathbf{A}\mathbf{x}\|_2} - \frac{\mathbf{A}^\top \mathbf{A}\mathbf{x}\mathbf{x}^\top \mathbf{A}^\top \mathbf{A}}{\|\mathbf{A}\mathbf{x}\|_2^3}.$$

Proof. Applying the rule for the derivative of a quotient of two differentiable functions, we get:

$$\frac{\partial}{\partial \mathbf{x}}\left(\frac{\mathbf{A}^\top \mathbf{A}\mathbf{x}}{\|\mathbf{A}\mathbf{x}\|_2}\right) = \frac{\mathbf{A}^\top \mathbf{A}\|\mathbf{A}\mathbf{x}\|_2}{\|\mathbf{A}\mathbf{x}\|_2^2} - \frac{\mathbf{A}^\top \mathbf{A}\mathbf{x}}{\|\mathbf{A}\mathbf{x}\|_2^2}\frac{\partial}{\partial \mathbf{x}}\sqrt{\|\mathbf{A}\mathbf{x}\|_2^2}$$

$$= \frac{\mathbf{A}^\top \mathbf{A}}{\|\mathbf{A}\mathbf{x}\|_2} - \frac{\mathbf{A}^\top \mathbf{A}\mathbf{x}}{\|\mathbf{A}\mathbf{x}\|_2^2}\frac{1}{2\|\mathbf{A}\mathbf{x}\|_2}2(\mathbf{A}^\top \mathbf{A}\mathbf{x})^\top,$$

which completes the proof. $\square$

Lemma 3. *Let* $\boldsymbol{u}, \boldsymbol{v} \in \mathbb{R}^n$ *with* $n \geq 2$, $\mathbf{u} \neq \mathbf{v}$, $a, b, c \in \mathbb{R} \setminus \{0\}$, *then the spectrum of the matrix:*

$$\boldsymbol{\Pi} = a\boldsymbol{I}_n + b\boldsymbol{u}\boldsymbol{u}^\top + c(\boldsymbol{u}\boldsymbol{v}^\top + \boldsymbol{v}\boldsymbol{u}^\top) \in \mathbb{S}^n,$$

is

$$\lambda_1 = \frac{1}{2}(2a + b\|\mathbf{u}\|_2^2 + 2c\mathbf{v}^\top\mathbf{u}) + \frac{1}{2}\sqrt{\Delta},$$

$$\lambda_2 = a, \qquad \textit{with multiplicity } n-2,$$

$$\lambda_3 = \frac{1}{2}(2a + b\|\mathbf{u}\|_2^2 + 2c\mathbf{v}^\top\mathbf{u}) - \frac{1}{2}\sqrt{\Delta},$$

and $\Delta = 4c^2\|\mathbf{u}\|_2^2\|\mathbf{v}\|_2^2 + b^2\|\mathbf{u}\|_2^4 + 4bc\|\mathbf{u}\|_2^2\mathbf{v}^\top\mathbf{u}$, *if* $n > 2$ *and* (λ_1, λ_3) *if* $n = 2$.

Proof. Let $\boldsymbol{M} = b\boldsymbol{u}\boldsymbol{u}^\top + c\left(\boldsymbol{u}\boldsymbol{v}^\top + \boldsymbol{v}\boldsymbol{u}^\top\right) \in \mathbb{S}^n$, then $\mathrm{rank}(\boldsymbol{M}) \leq \mathrm{rank}\left(b\boldsymbol{u}\boldsymbol{u}^\top\right) + \mathrm{rank}\left(c\left(\boldsymbol{u}\boldsymbol{v}^\top + \boldsymbol{v}\boldsymbol{u}^\top\right)\right)$ ≤ 3. This means that the image of $\mathbf{M}$ lies in $\mathcal{S} = \mathrm{span}\{\boldsymbol{u}, \boldsymbol{v}\} \subset \mathbb{R}^n$, which is a two-dimensional subspace. Moreover, adding $a\mathbf{I}_n$ simply shifts the eigenvalues and does not affect the rank, therefore $\mathrm{rank}(\boldsymbol{\Pi}) \leq 3$. For any $\boldsymbol{w} \in \mathcal{S}^\perp$, we have:

$$\boldsymbol{\Pi}\boldsymbol{w} = a\boldsymbol{w},$$

from which we find that $\lambda_2 = a$ is an eigenvalue of $\boldsymbol{\Pi}$, with multiplicity equal to $n-2$. We now compute the restriction of $\boldsymbol{\Pi}$ to the 2-dimensional subspace $\mathcal{S}$. Let:

$$\alpha = \frac{\boldsymbol{u}^\top\boldsymbol{v}}{\|\boldsymbol{u}\|_2}, \qquad \beta = \sqrt{\|\mathbf{v}\|_2^2 - \alpha^2},$$

we define an orthonormal basis $\{\mathbf{e}_1, \mathbf{e}_2\}$ for $\mathcal{S}$ as $\mathbf{e}_1 = \frac{\mathbf{u}}{\|\mathbf{u}\|_2}$ and decompose $\mathbf{v}$ as $\mathbf{v} = \alpha\mathbf{e}_1 + \beta\mathbf{e}_2$, where $\mathbf{e}_2 = \frac{\mathbf{v} - \alpha\mathbf{e}_1}{\beta}$. We express $\boldsymbol{\Pi}$ on the basis $\{\mathbf{e}_1, \mathbf{e}_2\}$, and we rewrite $\boldsymbol{\Pi}$ as:

$$\boldsymbol{\Pi} = a\boldsymbol{I}_n + b\|\mathbf{u}\|_2^2\mathbf{e}_1\mathbf{e}_1^\top + c\|\mathbf{u}\|_2(\mathbf{e}_1\mathbf{v}^\top + \mathbf{v}\mathbf{e}_1^\top),$$

and substituting the expression for $\mathbf{v} = \alpha\mathbf{e}_1 + \beta\mathbf{e}_2$, we get:

$$\boldsymbol{\Pi} = a\boldsymbol{I}_n + b\|\mathbf{u}\|_2^2\mathbf{e}_1\mathbf{e}_1^\top + c\|\mathbf{u}\|_2\left[\mathbf{e}_1(\alpha\mathbf{e}_1^\top + \beta\mathbf{e}_2^\top) + (\alpha\mathbf{e}_1 + \beta\mathbf{e}_2)\mathbf{e}_1^\top\right]$$

$$= a\boldsymbol{I}_n + br^2\mathbf{e}_1\mathbf{e}_1^\top + cr\left[2\alpha\mathbf{e}_1\mathbf{e}_1^\top + \beta(\mathbf{e}_1\mathbf{e}_2^\top + \mathbf{e}_2\mathbf{e}_1^\top)\right],$$

where $r = \|\boldsymbol{u}\|_2$. Therefore, on the orthonormal basis $\{\mathbf{e}_1, \mathbf{e}_2\}$, the restriction of $\boldsymbol{\Pi}$ to $\mathcal{S}$ has the matrix:

$$\boldsymbol{\Pi}_\mathcal{S} = \begin{bmatrix} a + br^2 + 2cr\alpha & cr\beta \\ cr\beta & a \end{bmatrix}.$$

To compute its eigenvalues of $\boldsymbol{\Pi}_\mathcal{S}$, we solve the characteristic polynomial:

$$\lambda^2 - \mathrm{trace}\left(\boldsymbol{\Pi}_\mathcal{S}\right)\lambda + |\boldsymbol{\Pi}_\mathcal{S}| = 0,$$

where

$$\mathrm{trace}\left(\boldsymbol{\Pi}_\mathcal{S}\right) = \left(a + br^2 + 2cr\alpha\right) + a = 2a + br^2 + 2cr\alpha$$

$$|\boldsymbol{\Pi}_\mathcal{S}| = \left(a + br^2 + 2cr\alpha\right)a - (cr\beta)^2 = a\left(a + br^2 + 2cr\alpha\right) - c^2r^2\beta^2,$$

and therefore

$$\lambda_{1,2} = \frac{1}{2}\left[\mathrm{trace}\left(\boldsymbol{\Pi}_\mathcal{S}\right) \pm \sqrt{\mathrm{trace}\left(\boldsymbol{\Pi}_\mathcal{S}\right)^2 - 4|\boldsymbol{\Pi}_\mathcal{S}|}\right].$$

The complete set of eigenvalues of $\boldsymbol{\Pi}$ is:

$$\lambda_1 = \frac{1}{2}(2a + br^2 + 2cr\alpha) + \frac{1}{2}\sqrt{\Delta},$$

$$\lambda_2 = a, \qquad \textit{with multiplicity } n-2,$$

$$\lambda_3 = \frac{1}{2}(2a + br^2 + 2cr\alpha) - \frac{1}{2}\sqrt{\Delta},$$

where $\Delta = \text{trace}\,(\boldsymbol{\Pi}_{\mathcal{S}})^2 - 4|\boldsymbol{\Pi}_{\mathcal{S}}| = 4c^2r^2(\alpha^2 + \beta^2) + b^2r^4 + 4bcr^3\alpha$. Substituting for the expression of r, α and β completes the proof. Concerning the case $n = 2$, the complete set of eigenvalues is (λ_1, λ_3) since $\mathcal{S}^\perp = \emptyset$. $\qquad\square$

Lemma 4. *Let $\boldsymbol{u}, \boldsymbol{v} \in \mathbb{R}^n$ with $n \geq 2$, $\gamma, w, r \in \mathbb{R}_+$, then the quantity*

$$\Delta = \frac{w^2}{\|\boldsymbol{u}\|_2^6}\left(-3\gamma^2(\boldsymbol{u}^\top\boldsymbol{v})^2 + 2\gamma\|\boldsymbol{u}\|_2^2(\boldsymbol{u}^\top\boldsymbol{v}) + 4\gamma^2\|\boldsymbol{u}\|_2^2\|\boldsymbol{v}\|_2^2 + \|\boldsymbol{u}\|_2^4\right) = \frac{w^2}{\|\boldsymbol{u}\|_2^6}\mathcal{Q}(\boldsymbol{u}^\top\boldsymbol{v}),$$

is positive for all real vectors $\boldsymbol{u}, \boldsymbol{v}$, and it is strictly positive unless $\rho_{u,v} = -1$ and $\gamma\|\boldsymbol{v}\|_2 = \|\boldsymbol{u}\|_2$.

Proof. Let $x = \boldsymbol{u}^\top\boldsymbol{v} \in \mathbb{R}$ and define $\mathcal{Q}(x) = -3\gamma^2x^2 + 2\gamma\|\boldsymbol{u}\|_2^2 x + 4\gamma^2\|\boldsymbol{u}\|_2^2\|\boldsymbol{v}\|_2^2 + \|\boldsymbol{u}\|_2^4$. By the Cauchy-Schwarz inequality, $|x| = |\boldsymbol{u}^\top\boldsymbol{v}| \leq \|\boldsymbol{u}\|_2\|\boldsymbol{v}\|_2$, then

$$\mathcal{Q}(x) \geq -3\gamma^2\|\boldsymbol{u}\|_2^2\|\boldsymbol{v}_g\|_2^2 + 2\gamma\|\boldsymbol{u}\|_2^2 x + 4\gamma^2\|\boldsymbol{u}\|_2^2\|\boldsymbol{v}\|_2^2 + \|\boldsymbol{u}\|_2^4$$
$$= \gamma^2\|\boldsymbol{u}\|_2^2\|\boldsymbol{v}\|_2^2 + 2\gamma\|\boldsymbol{u}\|_2^2 x + \|\boldsymbol{u}\|_2^4.$$

Since $-\|\boldsymbol{u}\|_2\|\boldsymbol{v}\|_2 \leq x \leq \|\boldsymbol{u}\|_2\|\boldsymbol{v}\|_2$, even in the worst-case $x = -\|\boldsymbol{u}\|_2\|\boldsymbol{v}\|_2$ or equivalently $\rho_{u,v} = -1$, we have:

$$\mathcal{Q}(\mathbf{u}^\top\mathbf{v}) \geq \gamma^2\|\boldsymbol{u}\|_2^2\|\boldsymbol{v}\|_2^2 - 2\gamma\|\boldsymbol{u}\|_2^3\|\boldsymbol{v}\|_2 + \|\boldsymbol{u}\|_2^4$$
$$= \|\boldsymbol{u}\|_2^2\left(\gamma^2\|\boldsymbol{v}\|_2^2 - 2\gamma\|\boldsymbol{u}\|_2\|\boldsymbol{v}\|_2 + \|\boldsymbol{u}\|_2^2\right)$$
$$= \|\boldsymbol{u}\|_2^2\left(\gamma\|\boldsymbol{v}\|_2 - \|\boldsymbol{u}\|_2\right)^2 \geq 0,$$

which completes the proof. $\qquad\square$

Lemma 5. *Let $\mathbf{A} \in \mathbb{R}^{n\times n}$ be a symmetric indefinite matrix, and let $\mathbf{B} \in \mathbb{R}^{n\times n}$ be symmetric and positive semi-definite. Then $\text{trace}(\mathbf{AB}) > 0$, if*

$$\sum_{i\,:\,\lambda_i>0}\lambda_i\mathbf{v}_i^\top\mathbf{B}\mathbf{v}_i > \sum_{i\,:\,\lambda_i<0}|\lambda_i|\mathbf{v}_i^\top\mathbf{B}\mathbf{v}_i,$$

where $\{\mathbf{v}_i\}$ is an orthonormal basis of eigenvectors and $\lambda_i \in \mathbb{R}$ are the corresponding eigenvalues of $\mathbf{A}$.

Proof. Since $\mathbf{A}$ is symmetric, it admits the spectral decomposition $\mathbf{A} = \sum_{i=1}^n \lambda_i\mathbf{v}_i\mathbf{v}_i^\top$ with orthonormal eigenvectors $\{\mathbf{v}_i\}$. Then,

$$\mathbf{AB} = \left(\sum_{i=1}^n \lambda_i\mathbf{v}_i\mathbf{v}_i^\top\right)\mathbf{B} = \sum_{i=1}^n \lambda_i\mathbf{v}_i(\mathbf{v}_i^\top\mathbf{B}),$$

and taking the trace:

$$\text{trace}(\mathbf{AB}) = \sum_{i=1}^n \lambda_i\text{trace}(\mathbf{v}_i\mathbf{v}_i^\top\mathbf{B}) = \sum_{i=1}^n \lambda_i\mathbf{v}_i^\top\mathbf{B}\mathbf{v}_i.$$

Now, separate the sum according to the sign of λ_i:

$$\text{trace}(\mathbf{AB}) = \sum_{i\,:\,\lambda_i>0}\lambda_i\mathbf{v}_i^\top\mathbf{B}\mathbf{v}_i + \sum_{i\,:\,\lambda_i<0}\lambda_i\mathbf{v}_i^\top\mathbf{B}\mathbf{v}_i.$$

Note that for $\lambda_i < 0$, we write $\lambda_i = -|\lambda_i|$, so:

$$\text{trace}(\mathbf{AB}) = \sum_{i\,:\,\lambda_i>0}\lambda_i\mathbf{v}_i^\top\mathbf{B}\mathbf{v}_i - \sum_{i\,:\,\lambda_i<0}|\lambda_i|\mathbf{v}_i^\top\mathbf{B}\mathbf{v}_i,$$

which is greater than zero, if and only if

$$\sum_{i\,:\,\lambda_i>0}\lambda_i\mathbf{v}_i^\top\mathbf{B}\mathbf{v}_i > \sum_{i\,:\,\lambda_i<0}|\lambda_i|\mathbf{v}_i^\top\mathbf{B}\mathbf{v}_i,$$

as required. $\qquad\square$