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Consistency of the Group Lasso and Multiple Kernel Learning

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Abstract

We consider the least-square regression problem with regularization by a block ℓ_1 -norm, i.e., a sum of Euclidean norms over spaces of dimensions larger than one. This problem, referred to as the group Lasso, extends the usual regularization by the ℓ_1 -norm where all spaces have dimension one, where it is commonly referred to as the Lasso. In this paper, we study the asymptotic model consistency of the group Lasso. We derive necessary and sufficient conditions for the consistency of group Lasso under practical assumptions, such as model misspecification. When the linear predictors and Euclidean norms are replaced by functions and reproducing kernel Hilbert norms, the problem is usually referred to as multiple kernel learning and is commonly used for learning from heterogeneous data sources and for non linear variable selection. Using tools from functional analysis, and in particular covariance operators, we extend the consistency results to this infinite dimensional case and also propose an adaptive scheme to obtain a consistent model estimate, even when the necessary condition required for the non adaptive scheme is not satisfied.

Keywords: Sparsity, regularization, consistency, convex optimization, covariance operators

1. Introduction

Regularization has emerged as a dominant theme in machine learning and statistics. It provides an intuitive and principled tool for learning from high-dimensional data. Regularization by squared Euclidean norms or squared Hilbertian norms has been thoroughly studied in various settings, from approximation theory to statistics, leading to efficient practical algorithms based on linear algebra and very general theoretical consistency results (Tikhonov and Arsenin, 1997, Wahba, 1990, Hastie et al., 2001, Steinwart, 2001, Cucker and Smale, 2002).

In recent years, regularization by non Hilbertian norms has generated considerable interest in linear supervised learning, where the goal is to predict a response as a linear function of covariates; in particular, regularization by the ℓ_1 -norm (equal to the sum of absolute values), a method commonly referred to as the *Lasso* (Tibshirani, 1994, Osborne et al., 2000), allows to perform variable selection. However, regularization by non Hilbertian norms cannot be solved empirically by simple linear algebra and instead leads to general convex optimization problems and much of the early effort has been dedicated to algorithms to solve the optimization problem efficiently. In particular, the *Lars* algorithm of Efron et al. (2004) allows to find the entire regularization path (i.e., the set of solutions for all values of the regularization parameters) at the cost of a single matrix inversion.

As the consequence of the optimality conditions, regularization by the ℓ_1 -norm leads to *sparse* solutions, i.e., loading vectors with many zeros. Recent works (Zhao and Yu, 2006, Yuan and Lin, 2007, Zou, 2006, Wainwright, 2006) have looked precisely at the model consistency of the Lasso, i.e., if we know that the data were generated from a sparse loading vector, does the Lasso actually recover it when the number of observed data points grows? In the case of a fixed number

of covariates, the Lasso does recover the sparsity pattern if and only if a certain simple condition on the generating covariance matrices is verified (Yuan and Lin, 2007). In particular, in low correlation settings, the Lasso is indeed consistent. However, in presence of strong correlations, the Lasso cannot be consistent, shedding light on potential problems of such procedures for variable selection. Adaptive versions where data-dependent weights are added to the ℓ_1 -norm then allow to keep the consistency in all situations (Zou, 2006).

A related Lasso-type procedure is the *group Lasso*, where the covariates are assumed to be clustered in groups, and instead of summing the absolute values of each individual loading, the sum of Euclidean norms of the loadings in each group is used. Intuitively, this should drive all the weights in one group to zero *together*, and thus lead to group selection (Yuan and Lin, 2006). In Section 2, we extend the consistency results of the Lasso to the group Lasso, showing that similar correlation conditions are necessary and sufficient conditions for consistency. The passage from groups of size one to groups of larger sizes leads however to a slightly weaker result as we can not get a single necessary and sufficient condition (in Section 2.4, we show that the stronger result similar to the Lasso is not true as soon as one group has dimension larger than one). Also, in our proofs, we relax the assumptions usually made for such consistency results, i.e., that the model is completely well-specified (conditional expectation of the response which is linear in the covariates and constant conditional variance). In the context of *misspecification*, which is a common situation when applying methods such as the ones presented in this paper, we simply prove convergence to the best linear predictor (which is assumed to be sparse), both in terms of loading vectors and sparsity patterns.

The group Lasso essentially replaces groups of size one by groups of size larger than one. It is natural in this context to allow the size of each group to grow unbounded, i.e., to replace the sum of Euclidean norms by a sum of appropriate Hilbertian norms. When the Hilbert spaces are reproducing kernel Hilbert spaces (RKHS), this procedure turns out to be equivalent to learn the best convex combination of a set of basis kernels, where each kernel corresponds to one Hilbertian norm used for regularization (Bach et al., 2004a). This framework, referred to as *multiple kernel learning* (Bach et al., 2004a), has applications in kernel selection, data fusion from heterogeneous data sources and non linear variable selection (Lanckriet et al., 2004a). In this latter case, multiple kernel learning can exactly be seen as variable selection in a *generalized additive model* (Hastie and Tibshirani, 1990). We extend the consistency results of the group Lasso to this non parametric case, by using covariance operators and appropriate notions of functional analysis. These notions allow to carry out the analysis entirely in “*primal/input*” space, while the algorithm has to work in “*dual/feature*” space to avoid infinite dimensional optimization. Throughout the paper, we will always go back and forth between primal and dual formulations, primal formulation for analysis and dual formulation for algorithms.

The paper is organized as follows: in Section 2, we present the consistency results for the group Lasso, while in Section 3, we extend these to Hilbert spaces. Finally, we present the adaptive schemes in Section 4 and illustrate our set of results with simulations on synthetic examples in Section 5.

2. Consistency of the Group Lasso

We consider the problem of predicting a response $Y \in \mathbb{R}$ from covariates $X \in \mathbb{R}^p$, where X has a block structure with m blocks, i.e., $X = (X_1^\top, \dots, X_m^\top)^\top$ with each $X_j \in \mathbb{R}^{p_j}$, $j = 1, \dots, m$,

and $\sum_{j=1}^m p_j = p$. Unless otherwise specified, $\|X\|$ will denote the Euclidean norm of a vector X . The only assumptions that we make on the joint distribution P_{XY} of (X, Y) are the following:

- (A1) X and Y have finite fourth order moments: $\mathbb{E}\|X\|^4 < \infty$ and $\mathbb{E}\|Y\|^4 < \infty$.
- (A2) The joint covariance matrix $\Sigma_{XX} = \mathbb{E}XX^\top - (\mathbb{E}X)(\mathbb{E}X)^\top \in \mathbb{R}^{p \times p}$ is invertible.
- (A3) We let $(\mathbf{w}, \mathbf{b}) \in \mathbb{R}^p \times \mathbb{R}$ denote any minimizer of $\mathbb{E}(Y - X^\top w - b)^2$. We assume that $\mathbb{E}((Y - \mathbf{w}^\top X - \mathbf{b})^2 | X)$ is almost surely greater than $\sigma_{\min}^2 > 0$. We let denote $\mathbf{J} = \{j, \mathbf{w}_j \neq 0\}$ the sparsity pattern of \mathbf{w} .¹

The assumption (A3) does not state that $\mathbb{E}(Y|X)$ is an affine function of X and that the conditional variance is constant, as it is commonly done in most works dealing with consistency for linear supervised learning. We simply assume that given the best affine predictor of Y given X (defined by $\mathbf{w} \in \mathbb{R}^p$ and $\mathbf{b} \in \mathbb{R}$), there is still a strictly positive amount of variance in Y . If (A2) is satisfied, then the full loading vector \mathbf{w} is uniquely defined and is equal to $\mathbf{w} = (\Sigma_{XX}^\top)^{-1} \Sigma_{XY}$, where $\Sigma_{XY} = \mathbb{E}(XY) - (\mathbb{E}X)(\mathbb{E}Y) \in \mathbb{R}^p$. Note that throughout this paper, we do include a non regularized constant term b but since we use a square loss it will be optimized out in closed form by centering the data. Thus all our consistency statements will be stated only for the loading vector w ; corresponding results for b then immediately follow.

We often use the notation $\varepsilon = Y - \mathbf{w}^\top X - \mathbf{b}$. In terms of covariance matrices, our assumption (A3) leads to: $\Sigma_{\varepsilon\varepsilon|X} = \mathbb{E}(\varepsilon\varepsilon|X) \geq \sigma_{\min}^2$ and $\Sigma_{\varepsilon X} = 0$ (but ε might not in general be independent from X).

Applications of grouped variables In this paper, we assume that the groupings of the univariate variables is known and fixed, i.e., the group structure is given and we wish to achieve sparsity at the level of groups. This has numerous applications, e.g., in speech and signal processing, where groups may represent different frequency bands (McAuley et al., 2005), or bioinformatics (Lanckriet et al., 2004a) and computer vision (Varma and Ray, 2007, Harchaoui and Bach, 2007) where each group may correspond to different data sources or data types. Note that those different data sources are sometimes referred to as *views* (see, e.g., Zhou and Burges, 2007).

Moreover, we always assume that the number m of groups is fixed and finite. Considering cases where m is allowed to grow with the number of observed data points, in the line of Meinshausen and Yu (2006), is outside the scope of this paper.

Notations Throughout this paper, we consider the block covariance matrix Σ_{XX} with m^2 blocks $\Sigma_{X_i X_j}$, $i, j = 1, \dots, m$. We refer to the submatrix composed of all blocks indexed by sets I, J as $\Sigma_{X_I X_J}$. Similarly, our loadings are vectors defined following block structure, $w = (w_1^\top, \dots, w_m^\top)^\top$ and we denote w_I the elements indexed by I . Moreover we denote $\mathbf{1}_q$ the vector in \mathbb{R}^q with constant components equal to one, and I_q the identity matrix of size q .

2.1 Group Lasso

We consider *independent and identically distributed* (i.i.d.) data $(x_i, y_i) \in \mathbb{R}^p \times \mathbb{R}$, $i = 1, \dots, n$, sampled from P_{XY} and the data are given in the form of matrices $\bar{Y} \in \mathbb{R}^n$ and $\bar{X} \in \mathbb{R}^{n \times p}$ and we write $\bar{X} = (\bar{X}_1, \dots, \bar{X}_m)$ where each $\bar{X}_j \in \mathbb{R}^{n \times p_j}$ represents the data associated with group j .

1. Note that throughout this paper, we use boldface fonts for population quantities.

Throughout this paper, we make the same i.i.d. assumption; dealing with non identically distributed or dependent data and extending our results in those situations are left for future research.

We consider the following optimization problem:

$$\min_{w \in \mathbb{R}^p, b \in \mathbb{R}} \frac{1}{2n} \|\bar{Y} - \bar{X}w - b\mathbf{1}_n\|^2 + \lambda_n \sum_{j=1}^m d_j \|w_j\|,$$

where $d \in \mathbb{R}^m$ is a vector of strictly positive fixed weights. Note that considering weights in the block ℓ_1 -norm is important in practice as those have an influence regarding the consistency of the estimator (see Section 4 for further details). Since b is not regularized, we can minimize in closed form with respect to b , by setting $b = \frac{1}{n} \mathbf{1}_n^\top (\bar{Y} - \bar{X}w)$. This leads to the following reduced optimization problem in w :

$$\min_{w \in \mathbb{R}^p} \frac{1}{2} \hat{\Sigma}_{YY} - \hat{\Sigma}_{XY}^\top w + \frac{1}{2} w^\top \hat{\Sigma}_{XX} w + \lambda_n \sum_{j=1}^m d_j \|w_j\|, \quad (1)$$

where $\hat{\Sigma}_{YY} = \frac{1}{n} \bar{Y}^\top \Pi_n \bar{Y}$, $\hat{\Sigma}_{XY} = \frac{1}{n} \bar{X}^\top \Pi_n \bar{Y}$ and $\hat{\Sigma}_{XX} = \frac{1}{n} \bar{X}^\top \Pi_n \bar{X}$ are empirical covariance matrices (with the centering matrix Π_n defined as $\Pi_n = I_n - \frac{1}{n} \mathbf{1}_n \mathbf{1}_n^\top$). We denote \hat{w} any minimizer of Eq. (1). We refer to \hat{w} as the *group Lasso* estimate². Note that with probability tending to one, if **(A2)** is satisfied (i.e., if Σ_{XX} is invertible), there is a unique minimum.

Problem (1) is a non-differentiable convex optimization problem, for which classical tools from convex optimization (Boyd and Vandenberghe, 2003) lead to the following optimality conditions (see proof by Yuan and Lin (2006) and in Appendix A.1):

Proposition 1 *A vector $w \in \mathbb{R}^p$ with sparsity pattern $J = J(w) = \{j, w_j \neq 0\}$ is optimal for problem (1) if and only if*

$$\forall j \in J^c, \quad \left\| \hat{\Sigma}_{X_j X} w - \hat{\Sigma}_{X_j Y} \right\| \leq \lambda_n d_j, \quad (2)$$

$$\forall j \in J, \quad \hat{\Sigma}_{X_j X} w - \hat{\Sigma}_{X_j Y} = -w_j \frac{\lambda_n d_j}{\|w_j\|}. \quad (3)$$

2.2 Algorithms

Efficient *exact* algorithms exist for the regular Lasso, i.e., for the case where all group dimensions p_j are equal to one. They are based on the piecewise linearity of the set of solutions as a function of the regularization parameter λ_n (Efron et al., 2004). For the group Lasso, however, the path is only piecewise differentiable, and following such a path is not as efficient as for the Lasso. Other algorithms have been designed to solve problem (1) for a single value of λ_n , in the original group Lasso setting (Yuan and Lin, 2006) and in the multiple kernel setting (Bach et al., 2004a,b, Sonnenburg et al., 2006, Rakotomamonjy et al., 2007). In this paper, we study path consistency of the group Lasso and of multiple kernel learning, and in simulations we use the publicly available code for the algorithm of Bach et al. (2004b), that computes an approximate but entire path, by following the piecewise smooth path with predictor-corrector methods.

2. We use the convention that all “hat” notations correspond to data-dependent and thus n -dependent quantities, so we do not need the explicit dependence on n .

2.3 Consistency Results

We consider the following two conditions:

$$\max_{i \in \mathbf{J}^c} \frac{1}{d_i} \left\| \Sigma_{X_i X_{\mathbf{J}}} \Sigma_{X_{\mathbf{J}} X_{\mathbf{J}}}^{-1} \text{Diag}(d_j / \|\mathbf{w}_j\|) \mathbf{w}_{\mathbf{J}} \right\| < 1, \quad (4)$$

$$\max_{i \in \mathbf{J}^c} \frac{1}{d_i} \left\| \Sigma_{X_i X_{\mathbf{J}}} \Sigma_{X_{\mathbf{J}} X_{\mathbf{J}}}^{-1} \text{Diag}(d_j / \|\mathbf{w}_j\|) \mathbf{w}_{\mathbf{J}} \right\| \leq 1, \quad (5)$$

where $\text{Diag}(d_j / \|\mathbf{w}_j\|)$ denotes the block-diagonal matrix (with block sizes p_j) in which each diagonal block is equal to $\frac{d_j}{\|\mathbf{w}_j\|} I_{p_j}$ (with I_{p_j} the identity matrix of size p_j), and $\mathbf{w}_{\mathbf{J}}$ denotes the concatenation of the loading vectors indexed by \mathbf{J} . Note that the conditions involve the covariance between all active groups $X_j, j \in \mathbf{J}$ and all non active groups $X_i, i \in \mathbf{J}^c$.

These are conditions on both the input (through the joint covariance matrix Σ_{XX}) and on the weight vector \mathbf{w} . Note that, when all blocks have size 1, this corresponds to the conditions derived for the Lasso (Zhao and Yu, 2006, Yuan and Lin, 2007, Zou, 2006). Note also the difference between the *strong condition* (4) and the *weak condition* (5). For the Lasso, with our assumptions, Yuan and Lin (2007) has shown that the strong condition (4) is necessary and sufficient for path consistency of the Lasso; i.e., the path of solutions consistently contains an estimate which is both consistent for the 2-norm (regular consistency) and the ℓ_0 -norm (consistency of patterns), if and only if condition (4) is satisfied.

In the case of the group Lasso, even with a finite fixed number of groups, our results are not as strong, as we can only get the strict condition as sufficient and the weak condition as necessary. In Section 2.4, we show that this cannot be improved in general. More precisely the following theorem, proved in Appendix B.1, shows that if the condition (4) is satisfied, any regularization parameter that satisfies a certain decay conditions will lead to a consistent estimator; thus the strong condition (4) is sufficient for path consistency:

Theorem 2 *Assume (A1-3). If condition (4) is satisfied, then for any sequence λ_n such that $\lambda_n \rightarrow 0$ and $\lambda_n n^{1/2} \rightarrow +\infty$, then the group Lasso estimate $\hat{\mathbf{w}}$ defined in Eq. (1) converges in probability to \mathbf{w} and the group sparsity pattern $J(\hat{\mathbf{w}}) = \{j, \hat{w}_j \neq 0\}$ converges in probability to \mathbf{J} (i.e., $\mathbb{P}(J(\hat{\mathbf{w}}) = \mathbf{J}) \rightarrow 1$).*

The following theorem, proved in Appendix B.2, states that if there is a consistent solution on the path, then the weak condition (5) must be satisfied.

Theorem 3 *Assume (A1-3). If there exists a (possibly data-dependent) sequence λ_n such that $\hat{\mathbf{w}}$ converges to \mathbf{w} and $J(\hat{\mathbf{w}})$ converges to \mathbf{J} in probability, then condition (5) is satisfied.*

On the one hand, Theorem 2 states that under the “low correlation between variables in \mathbf{J} and variables in \mathbf{J}^c ” condition (4), the group Lasso is indeed consistent. On the other hand, the result (and the similar one for the Lasso) is rather disappointing regarding the applicability of the group Lasso as a practical group selection method, as Theorem 3 states that if the weak correlation condition (5) is not satisfied, we cannot have consistency.

Moreover, this is to be contrasted with a thresholding procedure of the joint least-square estimator, which is also consistent with no conditions (but the invertibility of Σ_{XX}), if the threshold is

properly chosen (smaller than the smallest norm $\|\mathbf{w}_j\|$ for $j \in \mathbf{J}$ or with appropriate decay conditions). However, the Lasso and group Lasso do not have to set such a threshold; moreover, further analysis show that the Lasso has additional advantages over regular regularized least-square procedure (Meinshausen and Yu, 2006), and empirical evidence shows that in the finite sample case, they do perform better (Tibshirani, 1994), in particular in the case where the number m of groups is allowed to grow. In this paper we focus on the extension from uni-dimensional groups to multi-dimensional groups for finite number of groups m and leave the possibility of letting m grow with n for future research.

Finally, by looking carefully at condition (4) and (5), we can see that if we were to increase the weight d_j for $j \in \mathbf{J}^c$ and decrease the weights otherwise, we could always be consistent: this however requires the (potentially empirical) knowledge of \mathbf{J} and this is exactly the idea behind the adaptive scheme that we present in Section 4. Before looking at these extensions, we discuss in the next Section, qualitative differences between our results and the corresponding ones for the Lasso.

2.4 Refinements of Consistency Conditions

Our current results state that the strict condition (4) is sufficient for joint consistency of the group Lasso, while the weak condition (5) is only necessary. When all groups have dimension one, then the strict condition turns out to be also necessary (Yuan and Lin, 2007).

The main technical reason for those differences is that in dimension one, the set of vectors of unit norm is finite (two possible values), and thus regular squared norm consistency leads to estimates of the signs of the loadings (i.e., their normalized versions $\hat{w}_j/\|\hat{w}_j\|$) which are ultimately constant. When groups have size larger than one, then $\hat{w}_j/\|\hat{w}_j\|$ will not be ultimately constant (just consistent) and this added dependence on data leads to the following refinement of Theorem 2 (see proof in Appendix B.3):

Theorem 4 *Assume (A1-3). Assume the weak condition (5) is satisfied and that for all $i \in \mathbf{J}^c$ such that $\frac{1}{d_i} \left\| \Sigma_{X_i X_J} \Sigma_{X_J X_J}^{-1} \text{Diag}(d_j/\|\mathbf{w}_j\|) \mathbf{w}_J \right\| = 1$, we have*

$$\Delta^\top \Sigma_{X_J X_i} \Sigma_{X_i X_J} \Sigma_{X_J X_J}^{-1} \text{Diag} \left[d_j/\|\mathbf{w}_j\| \left(I_{p_j} - \frac{\mathbf{w}_j \mathbf{w}_j^\top}{\mathbf{w}_j^\top \mathbf{w}_j} \right) \right] \Delta > 0, \quad (6)$$

with $\Delta = -\Sigma_{X_J X_J}^{-1} \text{Diag}(d_j/\|\mathbf{w}_j\|) \mathbf{w}_J$. Then for any sequence λ_n such that $\lambda_n \rightarrow 0$ and $\lambda_n n^{1/4} \rightarrow +\infty$, then the group Lasso estimate \hat{w} defined in Eq. (1) converges in probability to \mathbf{w} and the group sparsity pattern $J(\hat{w}) = \{j, \hat{w}_j \neq 0\}$ converges in probability to \mathbf{J} .

This theorem is of lower practical significance than Theorem 2 and Theorem 3. It merely shows that the link between strict/weak conditions and sufficient/necessary conditions are in a sense tight (as soon as there exists $j \in \mathbf{J}$ such that $p_j > 1$, it is easy to exhibit examples where Eq. (6) is or is not satisfied). The previous theorem does not contradict the fact that condition (4) is necessary for path-consistency in the Lasso case: indeed, if w_j has dimension one, then $I_{p_j} - \frac{\mathbf{w}_j \mathbf{w}_j^\top}{\mathbf{w}_j^\top \mathbf{w}_j}$ is always equal to zero, and thus Eq. (6) is never satisfied. Note that when condition (6) is an equality, we could still refine the condition by using higher orders in the asymptotic expansions presented in Appendix B.3.

We can also further refined the *necessary* condition results in Theorem 3: as stated in Theorem 3, the group Lasso estimator may be both consistent in terms of norm and sparsity patterns only if the

condition (5) is satisfied. However, if we require only the consistent sparsity pattern estimation, then we may allow the convergence of the regularization parameter λ_n to a strictly positive limit λ_0 . In this situation, we may consider the following population problem:

$$\min_{\mathbf{w} \in \mathbb{R}^p} \frac{1}{2} (\mathbf{w} - \mathbf{w})^\top \Sigma_{XX} (\mathbf{w} - \mathbf{w}) + \lambda_0 \sum_{j=1}^m d_j \|\mathbf{w}_j\|. \quad (7)$$

If there exists $\lambda_0 > 0$ such that the solution has the correct sparsity pattern, then the group Lasso estimate with $\lambda_n \rightarrow \lambda_0$, will have a consistent sparsity pattern. The following proposition, which can be proved with standard M-estimation arguments, make this precise:

Proposition 5 *Assume (A1-3). If λ_n tends to $\lambda_0 > 0$, then the group Lasso estimate $\hat{\mathbf{w}}$ is sparsity-consistent if and only if the solution of Eq. (7) has the correct sparsity pattern.*

Thus, even when condition (5) is not satisfied, we may have consistent estimation of the sparsity pattern but inconsistent estimation of the loading vectors. We provide in Section 5 such examples.

2.5 Probability of Correct Pattern Selection

In this section, we focus on regularization parameters that tend to zero, at the rate $n^{-1/2}$, i.e., $\lambda_n = \lambda_0 n^{-1/2}$ with $\lambda_0 > 0$. For this particular setting, we can actually compute the limit of the probability of correct pattern selection (proposition proved in Appendix B.4). Note that in order to obtain a simpler result, we assume constant conditional variance of Y given $\mathbf{w}^\top X$:

Proposition 6 *Assume (A1-3) and $\text{var}(Y|\mathbf{w}^\top x) = \sigma^2$ almost surely. Assume moreover $\lambda_n = \lambda_0 n^{-1/2}$ with $\lambda_0 > 0$. Then, the group Lasso $\hat{\mathbf{w}}$ converges in probability to \mathbf{w} and the probability of correct sparsity pattern selection has the following limit:*

$$\mathbb{P} \left(\max_{i \in \mathcal{J}^c} \frac{1}{d_i} \left\| \frac{\sigma}{\lambda_0} t_i - \Sigma_{X_i X_{\mathcal{J}}} \Sigma_{X_{\mathcal{J}} X_{\mathcal{J}}}^{-1} \text{Diag} \left(\frac{d_j}{\|\mathbf{w}_j\|} \right) \mathbf{w}_{\mathcal{J}} \right\| \leq 1 \right), \quad (8)$$

where t is normally distributed with mean zero and covariance matrix $\Sigma_{X_{\mathcal{J}^c} X_{\mathcal{J}^c} | X_{\mathcal{J}}} = \Sigma_{X_{\mathcal{J}^c} X_{\mathcal{J}^c}} - \Sigma_{X_{\mathcal{J}^c} X_{\mathcal{J}}} \Sigma_{X_{\mathcal{J}} X_{\mathcal{J}}}^{-1} \Sigma_{X_{\mathcal{J}} X_{\mathcal{J}^c}}$ (which is the conditional covariance matrix of $X_{\mathcal{J}^c}$ given $X_{\mathcal{J}}$).

The previous theorem states that the probability of correct selection tends to the mass under a non degenerate multivariate distribution of the intersection of cylinders. Under our assumptions, this set is never empty and thus the limiting probability is strictly positive, i.e., there is (asymptotically) always a positive probability of estimating the correct pattern of groups.

Moreover, additional insights may be gained from Proposition 6, namely in terms of the dependence on σ , λ_0 and the tightness of the consistency conditions. First, when λ_0 tends to infinity, then the limit defined in Eq. (8) tends to one if the strict consistency condition (4) is satisfied, and tends to zero if one of the conditions is strictly not met. This corroborates the results of Theorem 2 and 3. Note however, that only an extension of Proposition 6 to λ_n that may deviate from a $n^{-1/2}$ would actually lead to a proof of Theorem 2, which is a subject of ongoing research.

Finally, Eq. (8) shows that σ has a smoothing effect on the probability of correct pattern selection, i.e., if condition (4) is satisfied, then this probability is a decreasing function of σ (and an increasing function of λ_0). Finally, the stricter the inequality in Eq. (4), the larger the probability of correct rank selection, which is illustrated in Section 5 on synthetic examples.

2.6 Loading Independent Sufficient Condition

Condition (4) depends on the loading vector \mathbf{w} and on the sparsity pattern \mathbf{J} , which are both a priori unknown. In this section, we consider sufficient conditions that do not depend on the loading vector, but only on the sparsity pattern \mathbf{J} and of course on the covariance matrices. The following condition is sufficient for consistency of the group Lasso, for all possible loading vectors \mathbf{w} with sparsity pattern \mathbf{J} :

$$C(\Sigma_{XX}, d, \mathbf{J}) = \max_{i \in \mathbf{J}^c} \max_{\forall j \in \mathbf{J}, \|u_j\|=1} \left\| \frac{1}{d_i} \Sigma_{X_i X_{\mathbf{J}}} \Sigma_{X_{\mathbf{J}} X_{\mathbf{J}}}^{-1} \text{Diag}(d_{\mathbf{J}}) u_{\mathbf{J}} \right\| < 1. \quad (9)$$

As opposed to the Lasso case, $C(\Sigma_{XX}, d, \mathbf{J})$ cannot be readily computed in closed form, but we have the following upper bound:

$$C(\Sigma_{XX}, d, \mathbf{J}) \leq \max_{i \in \mathbf{J}^c} \frac{1}{d_i} \sum_{j \in \mathbf{J}} d_j \left\| \sum_{k \in \mathbf{J}} \Sigma_{X_i X_k} \left(\Sigma_{X_{\mathbf{J}} X_{\mathbf{J}}}^{-1} \right)_{kj} \right\|,$$

where for a matrix M , $\|M\|$ denotes its maximal singular value (also known as its spectral norm). This leads to the following sufficient condition for consistency of the group Lasso (which extends the condition of Yuan and Lin, 2007):

$$\max_{i \in \mathbf{J}^c} \frac{1}{d_i} \sum_{j \in \mathbf{J}} d_j \left\| \sum_{k \in \mathbf{J}} \Sigma_{X_i X_k} \left(\Sigma_{X_{\mathbf{J}} X_{\mathbf{J}}}^{-1} \right)_{kj} \right\| < 1. \quad (10)$$

Given a set of weights d , better sufficient conditions than Eq. (10) may be obtained by solving a semidefinite programming problem (Boyd and Vandenberghe, 2003):

Proposition 7 *The quantity $\max_{\forall j \in \mathbf{J}, \|u_j\|=1} \left\| \Sigma_{X_i X_{\mathbf{J}}} \Sigma_{X_{\mathbf{J}} X_{\mathbf{J}}}^{-1} \text{Diag}(d_{\mathbf{J}}) u_{\mathbf{J}} \right\|^2$ is upperbounded by*

$$\max_{M \succcurlyeq 0, \text{tr} M_{ii} = 1} \text{tr} M \left(\text{Diag}(d_{\mathbf{J}}) \Sigma_{X_{\mathbf{J}} X_{\mathbf{J}}}^{-1} \Sigma_{X_{\mathbf{J}} X_i} \Sigma_{X_i X_{\mathbf{J}}} \Sigma_{X_{\mathbf{J}} X_{\mathbf{J}}}^{-1} \text{Diag}(d_{\mathbf{J}}) \right), \quad (11)$$

where M is a matrix defined by blocks following the block structure of $\Sigma_{X_{\mathbf{J}} X_{\mathbf{J}}}$. Moreover, the bound is also equal to

$$\min_{\lambda \in \mathbb{R}^m, \text{Diag}(d_{\mathbf{J}}) \Sigma_{X_{\mathbf{J}} X_{\mathbf{J}}}^{-1} \Sigma_{X_{\mathbf{J}} X_i} \Sigma_{X_i X_{\mathbf{J}}} \Sigma_{X_{\mathbf{J}} X_{\mathbf{J}}}^{-1} \text{Diag}(d_{\mathbf{J}}) \preceq \text{Diag}(\lambda)} \sum_{j=1}^m \lambda_j.$$

Proof We let denote $M = uu^{\top} \succcurlyeq 0$. Then if all u_j for $j \in \mathbf{J}$ have norm 1, then we have $\text{tr} M_{jj} = 1$ for all $j \in \mathbf{J}$. This implies the convex relaxation. The second problem is easily obtained as the convex dual of the first problem (Boyd and Vandenberghe, 2003). ■

Note that for the Lasso, the convex bound in Eq. (11) is tight and leads to the bound given above in Eq. (10) (Yuan and Lin, 2007, Wainwright, 2006). For the Lasso, Zhao and Yu (2006) consider several particular patterns of dependencies using Eq. (10). Note that this condition (and not the condition in Eq. (9)) is independent from the dimension and thus does not readily lead to rules of thumbs allowing to set the weight d_j as a function of the dimension p_j ; several rules of thumbs have been suggested, that loosely depend on the dimension on the blocks, in the context of the linear group Lasso (Yuan and Lin, 2006) or multiple kernel learning (Bach et al., 2004b); we argue in this paper, that weights should also depend on the response as well (see Section 4).

2.7 Alternative Formulation of the Group Lasso

Following Bach et al. (2004a), we can instead consider regularization by the square of the block ℓ_1 -norm:

$$\min_{w \in \mathbb{R}^p, b \in \mathbb{R}} \frac{1}{2n} \|\bar{Y} - \bar{X}w - b\mathbf{1}_n\|^2 + \frac{1}{2} \mu_n \left(\sum_{j=1}^m d_j \|w_j\| \right)^2.$$

This leads to the same path of solutions, but it is better behaved because each variable which is not zero is still regularized by the squared norm. The alternative version has also two advantages: (a) it has very close links to more general frameworks for learning the kernel matrix from data (Lanckriet et al., 2004b), and (b) it is essential in our proof of consistency in the functional case. We also get the equivalent formulation to Eq. (1), by minimizing in closed form with respect to b , to obtain:

$$\min_{w \in \mathbb{R}^p} \frac{1}{2} \hat{\Sigma}_{YY} - \hat{\Sigma}_{YX}w + \frac{1}{2} w^\top \hat{\Sigma}_{XX}w + \frac{1}{2} \mu_n \left(\sum_{j=1}^m d_j \|w_j\| \right)^2. \quad (12)$$

The following proposition gives the optimality conditions for the convex optimization problem defined in Eq. (12) (see proof in Appendix A.2):

Proposition 8 *A vector $w \in \mathbb{R}^p$ with sparsity pattern $J = \{j, w_j \neq 0\}$ is optimal for problem (12) if and only if*

$$\forall j \in J^c, \quad \left\| \hat{\Sigma}_{X_j X} w - \hat{\Sigma}_{X_j Y} \right\| \leq \mu_n d_j \left(\sum_{i=1}^n d_i \|w_i\| \right), \quad (13)$$

$$\forall j \in J, \quad \hat{\Sigma}_{X_j X} w - \hat{\Sigma}_{X_j Y} = -\mu_n \left(\sum_{i=1}^n d_i \|w_i\| \right) \frac{d_j w_j}{\|w_j\|}. \quad (14)$$

Note the correspondence at the optimum between optimal solutions of the two optimization problems in Eq. (1) and Eq. (12) through $\lambda_n = \mu_n \left(\sum_{i=1}^n d_i \|w_i\| \right)$. As far as consistency results are concerned, Theorem 3 immediately applies to the alternative formulation because the regularization paths are the same. For Theorem 2, it does not readily apply. But since the relationship between λ_n and μ_n at optimum is $\lambda_n = \mu_n \left(\sum_{i=1}^n d_i \|w_i\| \right)$ and that $\sum_{i=1}^n d_i \|\hat{w}_i\|$ converges to a constant whenever \hat{w} is consistent, it does apply as well with minor modifications (in particular, to deal with the case where \mathbf{J} is empty, which requires $\mu_n = \infty$).

3. Covariance Operators and Multiple Kernel Learning

We now extend the previous consistency results to the case of non-parametric estimation, where each group is a potentially infinite dimensional space of functions. Namely, the non parametric group Lasso aims at estimating a sparse linear combination of functions of separate random variables, and can then be seen as a variable selection method in a generalized additive model (Hastie and Tibshirani, 1990). Moreover, as shown in Section 3.5, the non-parametric group Lasso may also be seen as equivalent to learning a convex combination of kernels, a framework referred to as multiple kernel learning (MKL). In this context it is customary to have a single input space with several kernels (and hence Hilbert spaces) defined on the same input space (Lanckriet et al., 2004b, Bach et al., 2004a). Our framework accomodates this case as well, but our assumption **(A5)** regarding the

invertibility of the joint correlation operator states that the kernels cannot span Hilbert spaces which intersect.

In this nonparametric context, covariance operators constitute appropriate tools for the statistical analysis and are becoming standard in the theoretical analysis of kernel methods (Fukumizu et al., 2004, Gretton et al., 2005, Fukumizu et al., 2007, Caponnetto and de Vito, 2005). The following section reviews important concepts. For more details, see Baker (1973) and Fukumizu et al. (2004).

3.1 Review of Covariance Operator Theory

In this section, we first consider a single set \mathcal{X} and a positive definite kernel $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$, associated with the reproducing kernel Hilbert space (RKHS) \mathcal{F} of functions from \mathcal{X} to \mathbb{R} (see, e.g., Schölkopf and Smola (2001) or Berlinet and Thomas-Agnan (2003) for an introduction to RKHS theory). The Hilbert space and its dot product $\langle \cdot, \cdot \rangle_{\mathcal{F}}$ are such that for all $x \in \mathcal{X}$, then $k(\cdot, x) \in \mathcal{F}$ and for all $f \in \mathcal{F}$, $\langle k(\cdot, x), f \rangle_{\mathcal{F}} = f(x)$, which leads to the *reproducing property* $\langle k(\cdot, x), k(\cdot, y) \rangle_{\mathcal{F}} = k(x, y)$ for any $(x, y) \in \mathcal{X} \times \mathcal{X}$.

Covariance operator and norms Given a random variable X on \mathcal{X} with bounded second order moment, i.e., such that $\mathbb{E}k(X, X) < \infty$, we can define the covariance operator as the bounded linear operator Σ_{XX} from \mathcal{F} to \mathcal{F} such that for all $(f, g) \in \mathcal{F} \times \mathcal{F}$,

$$\langle f, \Sigma_{XX}g \rangle_{\mathcal{F}} = \text{cov}(f(X), g(X)) = \mathbb{E}(f(X)g(X)) - (\mathbb{E}f(X))(\mathbb{E}g(X)).$$

The operator Σ_{XX} is *auto-adjoint*, *non-negative* and *Hilbert-Schmidt*, i.e., for any orthonormal basis $(e_p)_{p \geq 1}$ of \mathcal{F} , then $\sum_{p=1}^{\infty} \|\Sigma_{XX}e_p\|_{\mathcal{F}}^2$ is finite; in this case, the value does not depend on the chosen basis and is referred to as the square of the Hilbert-Schmidt norm. The norm that we use by default in this paper is the operator norm $\|\Sigma_{XX}\|_{\mathcal{F}} = \sup_{f \in \mathcal{F}, \|f\|_{\mathcal{F}}=1} \|\Sigma_{XX}f\|_{\mathcal{F}}$, which is dominated by the Hilbert-Schmidt norm. Note that in the finite dimensional case where $\mathcal{X} = \mathbb{R}^p$, $p > 0$ and the kernel is linear, the covariance operator is exactly the covariance matrix, and the Hilbert-Schmidt norm is the Frobenius norm, while the operator norm is the maximum singular value (also referred to as the spectral norm).

The null space of the covariance operator is the space of functions $f \in \mathcal{F}$ such that $\text{var } f(X) = 0$, i.e., such that f is constant on the support of X .

Empirical estimators Given data $x_i \in \mathcal{X}, i = 1, \dots, n$ sampled i.i.d. from P_X , then the empirical estimate $\hat{\Sigma}_{XX}$ of Σ_{XX} is defined such that $\langle f, \hat{\Sigma}_{XX}g \rangle_{\mathcal{F}}$ is the empirical covariance between $f(X)$ and $g(X)$, which leads to:

$$\hat{\Sigma}_{XX} = \frac{1}{n} \sum_{i=1}^n k(\cdot, x_i) \otimes k(\cdot, x_i) - \frac{1}{n} \sum_{i=1}^n k(\cdot, x_i) \otimes \frac{1}{n} \sum_{i=1}^n k(\cdot, x_i),$$

where $u \otimes v$ is the operator defined by $\langle f, (u \otimes v)g \rangle_{\mathcal{F}} = \langle f, u \rangle_{\mathcal{F}} \langle g, v \rangle_{\mathcal{F}}$. If we further assume that the fourth order moment is finite, i.e., $\mathbb{E}k(X, X)^2 < \infty$, then the estimate is uniformly consistent i.e., $\|\hat{\Sigma}_{XX} - \Sigma_{XX}\|_{\mathcal{F}} = O_p(n^{-1/2})$ (see Fukumizu et al. (2007) and Appendix C.1), which generalizes the usual result of finite dimension.³

3. A random variable Z_n is said to be of order $O_p(a_n)$ if for any $\eta > 0$, there exists $M > 0$ such that $\sup_n \mathbb{P}(|Z_n| > Ma_n) < \eta$. See Van der Vaart (1998) for further definitions and properties of asymptotics in probability.

Cross-covariance and joint covariance operators Covariance operator theory can be extended to cases with more than one random variables (Baker, 1973). In our situation, we have m input spaces $\mathcal{X}_1, \dots, \mathcal{X}_m$ and m random variables $X = (X_1, \dots, X_m)$ and m RKHS $\mathcal{F}_1, \dots, \mathcal{F}_m$ associated with m kernels k_1, \dots, k_m .

If we assume that $\mathbb{E}k_j(X_j, X_j) < \infty$, for all $j = 1, \dots, m$, then we can naturally define the cross-covariance operators $\Sigma_{X_i X_j}$ from \mathcal{F}_j to \mathcal{F}_i such that $\forall (f_i, f_j) \in \mathcal{F}_i \times \mathcal{F}_j$,

$$\langle f_i, \Sigma_{X_i X_j} f_j \rangle_{\mathcal{F}_i} = \text{cov}(f_i(X_i), f_j(X_j)) = \mathbb{E}(f_i(X_i) f_j(X_j)) - (\mathbb{E}f_i(X_i))(\mathbb{E}f_j(X_j)).$$

These are also Hilbert-Schmidt operators, and if we further assume that $\mathbb{E}k_j(X_j, X_j)^2 < \infty$, for all $j = 1, \dots, m$, then the natural empirical estimators converges to the population quantities in Hilbert-Schmidt and operator norms at rate $O_p(n^{-1/2})$. We can now define a joint block covariance operator on $\mathcal{F} = \mathcal{F}_1 \times \dots \times \mathcal{F}_m$ following the block structure of covariance matrices in Section 2. As in the finite dimensional case, it leads to a joint covariance operator Σ_{XX} and we can refer to sub-blocks as $\Sigma_{X_I X_J}$ for the blocks indexed by I and J .

Moreover, we can define the bounded (i.e., with finite operator norm) correlation operators through $\Sigma_{X_i X_j} = \Sigma_{X_i X_i}^{1/2} C_{X_i X_j} \Sigma_{X_j X_j}^{1/2}$ (Baker, 1973). Throughout this paper we will make the assumption that those operators $C_{X_i X_j}$ are compact for $i \neq j$: compact operators can be characterized as limits of finite rank operators or as operators that can be diagonalized on a countable basis with spectrum composed of a sequence tending to zero (see, e.g., Brezis, 1980). This implies that the joint operator C_{XX} , naturally defined on $\mathcal{F} = \mathcal{F}_1 \times \dots \times \mathcal{F}_m$, is of the form ‘‘identity plus compact’’. It thus has a minimum and a maximum eigenvalue which are both between 0 and 1 (Brezis, 1980). If those eigenvalues are strictly greater than zero, then the operator is invertible, as are all the square sub-blocks. Moreover, the joint correlation operator is lower-bounded by a strictly positive constant times the identity operator.

Translation invariant kernels A particularly interesting ensemble of RKHS in the context of nonparametric estimation is the set of translation invariant kernels defined over $\mathcal{X} = \mathbb{R}^p$, where $p \geq 1$, of the form $k(x, x') = q(x' - x)$ where q is a function on \mathbb{R}^p with pointwise nonnegative integrable Fourier transform (which implies that q is continuous). In this case, the associated RKHS is $\mathcal{F} = \{q_{1/2} * g, g \in L^2(\mathbb{R}^p)\}$, where $q_{1/2}$ denotes the inverse Fourier transform of the square root of the Fourier transform of q and $*$ denotes the convolution operation, and $L^2(\mathbb{R}^p)$ denotes the space of square integrable functions. The norm is then equal to

$$\|f\|_{\mathcal{F}}^2 = \int \frac{|F(\omega)|^2}{Q(\omega)} d\omega,$$

where F and Q are the Fourier transforms of f and q (Wahba, 1990, Schölkopf and Smola, 2001). Functions in the RKHS are functions with appropriately integrable derivatives. In this paper, when using infinite dimensional kernels, we use the Gaussian kernel $k(x, x') = q(x - x') = \exp(-b\|x - x'\|^2)$.

One-dimensional Hilbert spaces In this paper, we also consider real random variables Y and ε embedded in the natural Euclidean structure of real numbers (i.e., we consider the linear kernel on \mathbb{R}). In this setting the covariance operator $\Sigma_{X_j Y}$ from \mathbb{R} to \mathcal{F}_j can be canonically identified as an element of \mathcal{F}_j . Throughout this paper, we always use this identification.

3.2 Problem Formulation

We assume in this section and in the remaining of the paper that for each $j = 1, \dots, m$, $X_j \in \mathcal{X}_j$ where \mathcal{X}_j is any set on which we have a reproducible kernel Hilbert spaces \mathcal{F}_j , associated with the positive kernel $k_j : \mathcal{X}_j \times \mathcal{X}_j \rightarrow \mathbb{R}$. We now make the following assumptions, that extends the assumptions **(A1)**, **(A2)** and **(A3)**. For each of them, we detail the main implications as well as common natural sufficient conditions. The first two conditions **(A4)** and **(A5)** depend solely on the input variables, while the two other ones, **(A6)** and **(A7)** consider the relationship between X and Y .

- (A4)** For each $j = 1 \dots, m$, \mathcal{F}_j is a separable reproducing kernel Hilbert space associated with kernel k_j , and the random variables $k_j(\cdot, X_j)$ are not constant and have finite fourth-order moments, i.e., $\mathbb{E}k_j(X_j, X_j)^2 < \infty$.

This is a non restrictive assumption in many situations; for example, when (a) $\mathcal{X}_j = \mathbb{R}^{p_j}$ and the kernel function (such as the Gaussian kernel) is bounded, or when (b) \mathcal{X}_j is a compact subset of \mathbb{R}^{p_j} and the kernel is any continuous function such as linear or polynomial. This implies notably, as shown in Section 3.1, that we can define covariance, cross-covariance and correlation operators that are all Hilbert-Schmidt (Baker, 1973, Fukumizu et al., 2007) and can all be estimated at rate $O_p(n^{-1/2})$ in operator norm.

- (A5)** All cross-correlation operators are compact and the joint correlation operator C_{XX} is invertible.

This is also a condition uniquely on the input spaces and not on Y . Following Fukumizu et al. (2007), a simple sufficient condition is that we have measurable spaces and distributions with joint density p_X (and marginal distributions $p_{X_i}(x_i)$ and $p_{X_i X_j}(x_i, x_j)$) and that the *mean square contingency* between all pairs of variables is finite, i.e.

$$\mathbb{E} \left\{ \frac{p_{X_i X_j}(x_i, x_j)}{p_{X_i}(x_i)p_{X_j}(x_j)} - 1 \right\} < \infty.$$

The contingency is a measure of statistical dependency (Renyi, 1959), and thus this sufficient condition simply states that two variables X_i and X_j cannot be too dependent. In the context of multiple kernel learning for heterogeneous data fusion, this corresponds to having sources which are heterogeneous enough. On top of compacity we impose the invertibility of the joint correlation operator; we use this assumption to make sure that the functions $\mathbf{f}_1, \dots, \mathbf{f}_m$ are unique. This ensures the non existence of any set of functions f_1, \dots, f_m in the closures of $\mathcal{F}_1, \dots, \mathcal{F}_m$, such that $\text{var } f_j(X_j) > 0$ and a linear combination is constant on the support of the random variables. In the context of generalized additive models, this assumption is referred to as the empty *concurvity space* assumption (Hastie and Tibshirani, 1990).

- (A6)** There exists functions $\mathbf{f} = (\mathbf{f}_1, \dots, \mathbf{f}_m) \in \mathcal{F} = \mathcal{F}_1 \times \dots \times \mathcal{F}_m$, $\mathbf{b} \in \mathbb{R}$, and a function \mathbf{h} of $X = (X_1, \dots, X_m)$ such that $\mathbb{E}(Y|X) = \sum_{j=1}^m \mathbf{f}_j(X_j) + \mathbf{b} + \mathbf{h}(X)$ with $\mathbb{E}h(X)^2 < \infty$, $\mathbb{E}h(X) = 0$ and $\mathbb{E}\mathbf{h}(X)\mathbf{f}_j(X_j) = 0$ for all $j = 1, \dots, m$ and $\mathbf{f}_j \in \mathcal{F}_j$. We assume that $\mathbb{E}((Y - \mathbf{f}(X) - \mathbf{b})^2|X)$ is almost surely greater than $\sigma_{\min}^2 > 0$ and smaller than $\sigma_{\max}^2 < \infty$. We let denote $\mathbf{J} = \{j, \mathbf{f}_j \neq 0\}$ the sparsity pattern of \mathbf{f} .

This assumption on the conditional expectation of Y given X is not the most general and follows common assumptions in approximation theory (see, e.g., Caponnetto and de Vito (2005), Cucker and Smale (2002) and references therein). It allows misspecification, but it essentially requires that the conditional expectation of Y given sums of measurable functions of X_j is attained at functions in the RKHS, and not merely measurable functions. Dealing with more general assumptions in the line of Ravikumar et al. (2008) requires to consider consistency for norms weaker than the RKHS norms (Caponnetto and de Vito, 2005, Steinwart, 2001), and is left for future research. Note also, that to simplify proofs, we assume a finite upper-bound σ_{\max}^2 on the residual variance.

(A7) For all $j \in \{1, \dots, m\}$, there exists $\mathbf{g}_j \in \mathcal{F}_j$ such that $\mathbf{f}_j = \Sigma_{X_j X_j}^{1/2} \mathbf{g}_j$, i.e., each \mathbf{f}_j is in the range of $\Sigma_{X_j X_j}^{1/2}$.

This technical condition, already used by Caponnetto and de Vito (2005), which concerns all RKHS independently, ensures that we obtain consistency for the norm of the RKHS (and not another weaker norm) for the least-squares estimates. Note also that it implies that $\text{var } f_j(X_j) > 0$, i.e., f_j is not constant on the support of X_j .

This assumption might be checked (at least) in two ways; first, if $(e_p)_{p \geq 1}$ is a sequence of eigenfunctions of $\Sigma_{X X}$, associated with strictly positive eigenvalues $\lambda_p > 0$, then f is in the range of $\Sigma_{X X}$ if and only if f is constant outside the support of the random variable X and $\sum_{p \geq 1} \frac{1}{\lambda_p} \langle f, e_p \rangle^2$ is finite (i.e, the decay of the sequence $\langle f, e_p \rangle^2$ is strictly faster than λ_p).

We also provide another sufficient condition that sheds additional light on this technical condition which is always true for finite dimensional Hilbert spaces. For the common situation where $\mathcal{X}_j = \mathbb{R}^{p_j}$, P_{X_j} (the marginal distribution of X_j) has a density $p_{X_j}(x_j)$ with respect to the Lebesgue measure and the kernel is of the form $k_j(x_j, x'_j) = q_j(x_j - x'_j)$, we have the following proposition (proved in Appendix D.4):

Proposition 9 *Assume $\mathcal{X} = \mathbb{R}^p$ and X is a random variable on \mathcal{X} with distribution P_X that has a strictly positive density $p_X(x)$ with respect to the Lebesgue measure. Assume $k(x, x') = q(x - x')$ for a function $q \in L^2(\mathbb{R}^p)$ has an integrable pointwise positive Fourier transform, with associated RKHS \mathcal{F} . If f can be written as $f = q * g$ (convolution of q and g) with $\int_{\mathbb{R}^p} g(x) dx = 0$ and $\int_{\mathbb{R}^p} \frac{g(x)^2}{p_X(x)} dx < \infty$, then $f \in \mathcal{F}$ is in the range of the square root $\Sigma_{X X}^{1/2}$ of the covariance operator.*

The previous proposition gives natural conditions regarding f and p_X . Indeed, the condition $\int \frac{g(x)^2}{p_X(x)} dx < \infty$ corresponds to a natural support condition, i.e., f should be zero where X has no mass, otherwise, we will not be able to estimate f ; note the similarity with the usual condition regarding the variance of importance sampling estimation (Brémaud, 1999). Moreover, f should be even smoother than a regular function in the RKHS (convolution by q instead of the square root of q). Finally, we provide in Appendix E detailed covariance structures for Gaussian kernels with Gaussian variables.

Notations Throughout this section, we refer to functions $f = (f_1, \dots, f_m) \in \mathcal{F} = \mathcal{F}_1 \times \dots \times \mathcal{F}_m$ and the joint covariance operator $\Sigma_{X X}$. In the following, we always use the norms of the RKHS. When considering operators, we use the operator norm. We also refer to a subset of f indexed by J through f_J . Note that the Hilbert norm $\|f_J\|_{\mathcal{F}_J}$ is equal to $\|f_J\|_{\mathcal{F}_J} = (\sum_{j \in J} \|f_j\|_{\mathcal{F}_j})^{1/2}$. Finally, given a nonnegative auto-adjoint operator S , we let denote $S^{1/2}$ its nonnegative autoadjoint square root (Baker, 1973).

3.3 Nonparametric Group Lasso

Given i.i.d data (x_{ij}, y_i) , $i = 1, \dots, n$, $j = 1, \dots, m$, where each $x_{ij} \in \mathcal{X}_j$, our goal is to estimate consistently the functions \mathbf{f}_j and which of them are zero. We let denote $\bar{Y} \in \mathbb{R}^n$ the vector of responses. We consider the following optimization problem:

$$\min_{f \in \mathcal{F}, b \in \mathbb{R}} \frac{1}{2n} \sum_{i=1}^n \left(y_i - \sum_{j=1}^m f_j(x_{ij}) - b \right)^2 + \frac{\mu_n}{2} \left(\sum_{j=1}^m d_j \|f_j\|_{\mathcal{F}_j} \right)^2.$$

By minimizing with respect to b in closed form, we obtain a similar formulation to Eq. (12), where empirical covariance matrices are replaced by empirical covariance operators:

$$\min_{f \in \mathcal{F}} \frac{1}{2} \hat{\Sigma}_{YY} - \langle f, \hat{\Sigma}_{XY} \rangle_{\mathcal{F}} + \frac{1}{2} \langle f, \hat{\Sigma}_{XX} f \rangle_{\mathcal{F}} + \frac{\mu_n}{2} \left(\sum_{j=1}^m d_j \|f_j\|_{\mathcal{F}_j} \right)^2. \quad (15)$$

We let denote \hat{f} any minimizer of Eq. (15), and we refer to it as the non parametric group Lasso estimate, or also the multiple kernel learning estimate. By Proposition 13, the previous problem has indeed minimizers, and by Proposition 14 this global minimum is unique with probability tending to one.

Note that formally, the finite and infinite dimensional formulations in Eq. (12) and Eq. (15) are the same, and this is the main reason why covariance operators are very practical tools for the analysis. Furthermore, we have the corresponding proposition regarding optimality conditions (see proof in Appendix A.3):

Proposition 10 *A function $f \in \mathcal{F}$ with sparsity pattern $J = J(f) = \{j, f_j \neq 0\}$ is optimal for problem (15) if and only if*

$$\forall j \in J^c, \quad \left\| \hat{\Sigma}_{X_j X} f - \hat{\Sigma}_{X_j Y} \right\|_{\mathcal{F}_j} \leq \mu_n d_j \left(\sum_{i=1}^n d_i \|f_i\|_{\mathcal{F}_i} \right), \quad (16)$$

$$\forall j \in J, \quad \hat{\Sigma}_{X_j X} f - \hat{\Sigma}_{X_j Y} = -\mu_n \left(\sum_{i=1}^n d_i \|f_i\|_{\mathcal{F}_i} \right) \frac{d_j f_j}{\|f_j\|_{\mathcal{F}_j}}. \quad (17)$$

A consequence (and in fact the first part of the proof) is that an optimal function f must be in the range of $\hat{\Sigma}_{XY}$ and $\hat{\Sigma}_{XX}$, i.e., an optimal f is supported by the data; that is, each f_j is a linear combination of functions $k_j(\cdot, x_{ij})$, $i = 1, \dots, n$. This is a rather circumvolved way of presenting the representer theorem (Wahba, 1990), but this is the easiest for the theoretical analysis of consistency. However, to actually compute the estimate \hat{f} from data, we need the usual formulation with dual parameters (see Section 3.5).

Moreover, one important conclusion is that all our optimization problems in spaces of functions can be in fact transcribed into finite-dimensional problems. In particular, all notions from multivariate differentiable calculus may be used without particular care regarding the infinite dimension.

3.4 Consistency Results

We consider the following strict and weak conditions, which correspond to condition (4) and (5) in the finite dimensional case:

$$\max_{i \in \mathbf{J}^c} \frac{1}{d_i} \left\| \Sigma_{X_i X_i}^{1/2} C_{X_i X_{\mathbf{J}}} C_{X_{\mathbf{J}} X_{\mathbf{J}}}^{-1} \text{Diag}(d_j / \|f_j\|_{\mathcal{F}_j}) \mathbf{g}_{\mathbf{J}} \right\|_{\mathcal{F}_i} < 1, \quad (18)$$

$$\max_{i \in \mathbf{J}^c} \frac{1}{d_i} \left\| \Sigma_{X_i X_i}^{1/2} C_{X_i X_{\mathbf{J}}} C_{X_{\mathbf{J}} X_{\mathbf{J}}}^{-1} \text{Diag}(d_j / \|\mathbf{f}_j\|_{\mathcal{F}_j}) \mathbf{g}_{\mathbf{J}} \right\|_{\mathcal{F}_i} \leq 1, \quad (19)$$

where $\text{Diag}(d_j / \|\mathbf{f}_j\|_{\mathcal{F}_j})$ denotes the block-diagonal operator with operators $\frac{d_j}{\|\mathbf{f}_j\|_{\mathcal{F}_j}} I_{\mathcal{F}_j}$ on the diagonal. Note that this is well-defined because $C_{X_{\mathbf{J}} X_{\mathbf{J}}}$ is invertible and that it reduces to Eq. (4) and Eq. (5) when the input spaces \mathcal{X}_j , $j = 1, \dots, m$ are of the form \mathbb{R}^{p_j} and the kernels are linear. The main reason is rewriting the conditions in terms of correlation operators rather than covariance operators is that correlation operators are invertible by assumption, while covariance operators are not as soon as the Hilbert spaces have infinite dimensions. The following theorems give necessary and sufficient conditions for the path consistency of the nonparametric group Lasso (see proofs in Appendix C.2 and Appendix C.3):

Theorem 11 *Assume (A4-7) and that \mathbf{J} is not empty. If condition (18) is satisfied, then for any sequence μ_n such that $\mu_n \rightarrow 0$ and $\mu_n n^{1/2} \rightarrow +\infty$, any sequence of nonparametric group Lasso estimates $\hat{\mathbf{f}}$ converges in probability to \mathbf{f} and the sparsity pattern $J(\hat{\mathbf{f}}) = \{j, \hat{f}_j \neq 0\}$ converges in probability to \mathbf{J} .*

Theorem 12 *Assume (A4-7) and that \mathbf{J} is not empty. If there exists a (possibly data-dependent) sequence μ_n such $\hat{\mathbf{f}}$ converges to \mathbf{f} and $\hat{\mathbf{J}}$ converges to \mathbf{J} in probability, then condition (19) is satisfied.*

Essentially, the results in finite dimension also hold when groups have infinite dimensions. We leave the extensions of the refined results in Section 2.4 to future work. Condition (18) might be hard to check in practice since it involves inversion of correlation operators; see Section 3.6 for an estimate from data.

3.5 Multiple Kernel Learning Formulation

Proposition 10 does not readily lead to an algorithm for computing the estimate $\hat{\mathbf{f}}$. In this section, following Bach et al. (2004a), we link the group Lasso to the multiple kernel learning framework (Lanckriet et al., 2004b). Problem (15) is an optimization problem on a potentially infinite dimensional space of functions. However, the following proposition shows that it reduces to a finite dimensional problem that we now precise (see proof in Appendix A.4):

Proposition 13 *The dual of problem (15) is*

$$\max_{\alpha \in \mathbb{R}^n, \alpha^\top \mathbf{1}_n = 0} \left\{ -\frac{1}{2n} \|\bar{Y} - n\mu_n \alpha\|^2 - \frac{1}{2\mu_n} \max_{i=1, \dots, m} \frac{\alpha^\top K_i \alpha}{d_i^2} \right\}, \quad (20)$$

where $(K_i)_{ab} = k_i(x_a, x_b)$ are the kernel matrices in $\mathbb{R}^{n \times n}$, for $i = 1, \dots, m$. Moreover, the dual variable $\alpha \in \mathbb{R}^n$ is optimal if and only if $\alpha^\top \mathbf{1}_n = 0$ and there exists $\eta \in \mathbb{R}_+^m$ such that $\sum_{j=1}^m \eta_j d_j^2 = 1$ and

$$\left(\sum_{j=1}^m \eta_j K_j + n\mu_n I_n \right) \alpha = \bar{Y}, \quad (21)$$

$$\forall j \in \{1, \dots, m\}, \frac{\alpha^\top K_j \alpha}{d_j^2} < \max_{i=1, \dots, m} \frac{\alpha^\top K_i \alpha}{d_i^2} \Rightarrow \eta_j = 0. \quad (22)$$

The optimal function may then be written as $f_j = \eta_j \sum_{i=1}^n \alpha_i k_j(\cdot, x_{ij})$.

Since the problem in Eq. (20) is strictly convex, there is a unique dual solution α . Note that Eq. (21) corresponds to the optimality conditions for the least-square problem:

$$\min_{f \in \mathcal{F}} \frac{1}{2} \hat{\Sigma}_{YY} - \langle f, \hat{\Sigma}_{XY} \rangle_{\mathcal{F}} + \frac{1}{2} \langle f, \hat{\Sigma}_{XX} f \rangle_{\mathcal{F}} + \frac{1}{2} \mu_n \sum_{j, \eta_j > 0} \frac{\|f_j\|_{\mathcal{F}_j}^2}{\eta_j},$$

whose dual problem is:

$$\max_{\alpha \in \mathbb{R}^n, \alpha^\top \mathbf{1}_n = 0} \left\{ -\frac{1}{2n} \|\bar{Y} - n\mu_n \alpha\|^2 - \frac{1}{2\mu_n} \alpha^\top \left(\sum_{j=1}^m \eta_j K_j \right) \alpha \right\},$$

and unique solution is $\alpha = (\sum_{j=1}^m \eta_j K_j + n\mu_n I_n)^{-1} \bar{Y}$. That is, the solution of the MKL problem leads to dual parameters α and set of weights $\eta \geq 0$ such that α is the solution to the least-square problem with kernel $K = \sum_{j=1}^m \eta_j K_j$. Bach et al. (2004a) has shown in a very similar context (hinge loss instead of the square loss) that the optimal η in Proposition 13 can be obtained as the minimizer of the optimal value of the regularized least-square problem with kernel matrix $\sum_{j=1}^m \eta_j K_j$, i.e.:

$$J(\eta) = \max_{\alpha \in \mathbb{R}^n, \alpha^\top \mathbf{1}_n = 0} \left\{ -\frac{1}{2n} \|\bar{Y} - n\mu_n \alpha\|^2 - \frac{1}{2\mu_n} \alpha^\top \left(\sum_{j=1}^m \eta_j K_j \right) \alpha \right\},$$

with respect to $\eta \geq 0$ such that $\sum_{j=1}^m \eta_j d_j^2 = 1$. This formulation allows to derive probably approximately correct error bounds (Lanckriet et al., 2004b, Bousquet and Herrmann, 2003). Besides, this formulation allows η to be negative, as long as the matrix $\sum_{j=1}^m \eta_j K_j$ is positive semi-definite. However, theoretical advantages of such a possibility still remain unclear.

Finally, we state a corollary of Proposition 13 that shows that under our assumptions regarding the correlation operator, we have a unique solution to the non parametric groups Lasso problem with probability tending to one (see proof in Appendix A.5):

Proposition 14 *Assume (A4-5). The problem (15) has a unique solution with probability tending to one.*

3.6 Estimation of Correlation Condition (18)

Condition (4) is simple to compute while the non parametric condition (18) might be hard to check even if all densities are known (we provide however in Section 5 a specific example where we can compute in closed form all covariance operators). The following proposition shows that we can consistently estimate the quantities $\left\| \Sigma_{X_i X_i}^{1/2} C_{X_i X_J} C_{X_J X_J}^{-1} \text{Diag}(d_j / \|\mathbf{f}_j\|_{\mathcal{F}_j}) \mathbf{g}_J \right\|_{\mathcal{F}_i}$ given an i.i.d. sample (see proof in Appendix C.4):

Proposition 15 *Assume (A4-7), and $\kappa_n \rightarrow 0$ and $\kappa_n n^{1/2} \rightarrow \infty$. Let*

$$\alpha = \Pi_n \left(\sum_{j \in \mathbf{J}} \Pi_n K_j \Pi_n + n\kappa_n I_n \right)^{-1} \Pi_n \bar{Y}$$

and $\hat{\eta}_j = \frac{1}{d_j}(\alpha^\top K_j \alpha)^{1/2}$. Then, for all $i \in \mathbf{J}^c$, the norm $\left\| \Sigma_{X_i X_i}^{1/2} C_{X_i X_{\mathbf{J}}} C_{X_{\mathbf{J}} X_{\mathbf{J}}}^{-1} \text{Diag}(d_j / \|\mathbf{f}_j\|) \mathbf{g}_{\mathbf{J}} \right\|_{\mathcal{F}_i}$ is consistently estimated by:

$$\left\| (\Pi_n K_i \Pi_n)^{1/2} \left(\sum_{j \in \mathbf{J}} \Pi_n K_j \Pi_n + n \kappa_n I_n \right)^{-1} \left(\sum_{j \in \mathbf{J}} \frac{1}{\hat{\eta}_j} \Pi_n K_j \Pi_n \right) \alpha \right\|. \quad (23)$$

4. Adaptive Group Lasso and Multiple Kernel Learning

In previous sections, we have shown that specific necessary and sufficient conditions are needed for path consistency of the group Lasso and multiple kernel learning. The following procedures, adapted from the adaptive Lasso of Zou (2006), lead to two-step procedures that always achieve both consistency, with no condition such as Eq. (4) or Eq. (18). As before, results are a bit different when groups have finite sizes and groups may have infinite sizes.

4.1 Adaptive Group Lasso

The following theorem extends the similar theorem of Zou (2006), and shows that we can get both $O_p(n^{-1/2})$ consistency and correct pattern estimation:

Theorem 16 Assume (A1-3) and $\gamma > 0$. Let $\hat{w}^{LS} = \hat{\Sigma}_{XX}^{-1} \hat{\Sigma}_{XY}$ denote the (unregularized) least-square estimate. Let \hat{w}^A denote any minimizer of

$$\frac{1}{2} \hat{\Sigma}_{YY} - \hat{\Sigma}_{YX} w + \frac{1}{2} w^\top \hat{\Sigma}_{XX} w + \frac{\mu_n}{2} \left(\sum_{j=1}^m \|\hat{w}_j^{LS}\|^{-\gamma} \|w_j\| \right)^2.$$

If $n^{-1/2} \gg \mu_n \gg n^{-1/2-\gamma/2}$, then \hat{w}^A converges in probability to \mathbf{w} , $J(\hat{w}^A)$ converges in probability to \mathbf{J} , and $n^{1/2}(\hat{w}_{\mathbf{J}}^A - \mathbf{w}_{\mathbf{J}})$ tends in distribution to a normal distribution with mean zero and covariance matrix $\Sigma_{X_{\mathbf{J}} X_{\mathbf{J}}}^{-1}$.

This theorem, proved in Appendix D.1, shows that the adaptive group Lasso exhibit all important asymptotic properties, both in terms of errors and selected models. In the nonparametric case, we obtain a weaker result.

4.2 Adaptive Multiple Kernel Learning

We first begin with the consistency of the least-square estimate (see proof in Appendix D.2):

Proposition 17 Assume (A4-7). The unique minimizer $\hat{f}_{\kappa_n}^{LS}$ of

$$\frac{1}{2} \hat{\Sigma}_{YY} - \langle \hat{\Sigma}_{XY}, f \rangle_{\mathcal{F}} + \frac{1}{2} \langle f, \hat{\Sigma}_{XX} f \rangle_{\mathcal{F}} + \frac{\kappa_n}{2} \sum_{j=1}^m \|f_j\|_{\mathcal{F}_j}^2,$$

converges in probability to f if $\kappa_n \rightarrow 0$ and $\kappa_n n^{1/2} \rightarrow 0$. Moreover, we have $\|\hat{f}_{\kappa_n}^{LS} - f\|_{\mathcal{F}} = O_p(\kappa_n^{1/2} + \kappa_n^{-1} n^{-1/2})$.

Since the least-square estimate is consistent and we have an upper bound on its convergence rate, we follow Zou (2006) and use it to defined adaptive weights d_j for which we get both sparsity and regular consistency without any conditions on the value of the correlation operators.

Theorem 18 *Assume (A4-7) and $\gamma > 1$. Let $\hat{f}_{n^{-1/3}}^{LS}$ be the least-square estimate with regularization parameter proportional to $n^{-1/3}$, as defined in Proposition 17. Let \hat{f}^A denote any minimizer of*

$$\frac{1}{2} \hat{\Sigma}_{YY} - \langle \hat{\Sigma}_{XY}, f \rangle_{\mathcal{F}} + \frac{1}{2} \langle f, \hat{\Sigma}_{XX} f \rangle_{\mathcal{F}} + \frac{\mu_0 n^{-1/3}}{2} \left(\sum_{j=1}^m \|(\hat{f}_{\kappa_n}^{LS})_j\|_{\mathcal{F}_j}^{-\gamma} \|f_j\|_{\mathcal{F}_j} \right)^2.$$

Then \hat{f}^A converges to \mathbf{f} and $J(\hat{f}^A)$ converges to \mathbf{J} in probability.

Theorem 18 allows to set up a specific vector of weights d . This provides a principled way to define data adaptive weights, that allows to solve (at least theoretically) the potential consistency problems of the usual MKL framework (see Section 5 for illustration on synthetic examples). Note that we have no result concerning the $O_p(n^{-1/2})$ consistency of our procedure (as we have for the finite dimensional case) and obtaining precise convergence rates is the subject of ongoing research.

The following proposition gives the expression for the solution of the least-square problem, necessary for the computation of adaptive weights in Theorem 18.

Proposition 19 *The solution of the least-square problem in Proposition 17 is given by*

$$\forall j \in \{1, \dots, m\}, f_j^{LS} = \sum_{i=1}^n \alpha_i k_j(\cdot, x_{ij}) \text{ with } \alpha = \Pi_n \left(\sum_{j=1}^m \Pi_n K_j \Pi_n + n \kappa_n I_n \right)^{-1} \Pi_n \bar{Y},$$

with norms $\|\hat{F}_j^{LS}\|_{\mathcal{F}_j} = (\alpha^\top K_j \alpha)^{1/2}$, $j = 1, \dots, m$.

Other weighting schemes have been suggested, based on various heuristics. A notable one (which we use in simulations) is the normalization of kernel matrices by their trace (Lanckriet et al., 2004b), which leads to $d_j = (\text{tr} \hat{\Sigma}_{X_j X_j})^{1/2} = (\frac{1}{n} \text{tr} \Pi_n K_j \Pi_n)^{1/2}$. Bach et al. (2004b) have observed empirically that such normalization might lead to suboptimal solutions and consider weights d_j that grow with the empirical ranks of the kernel matrices. In this paper, we give theoretical arguments that indicate that weights which do depend on the data are more appropriate and work better (see Section 5 for examples).

5. Simulations

In this section, we illustrate the consistency results obtained in this paper with a few simple simulations on synthetic examples.

5.1 Groups of Finite Sizes

In the finite dimensional group case, we sampled $X \in \mathbb{R}^p$ from a normal distribution with zero mean vector and a covariance matrix of size $p = 8$ for $m = 4$ groups of size $p_j = 2$, $j = 1, \dots, m$, generated as follows: (a) sample an $p \times p$ matrix G with independent standard normal distributions,

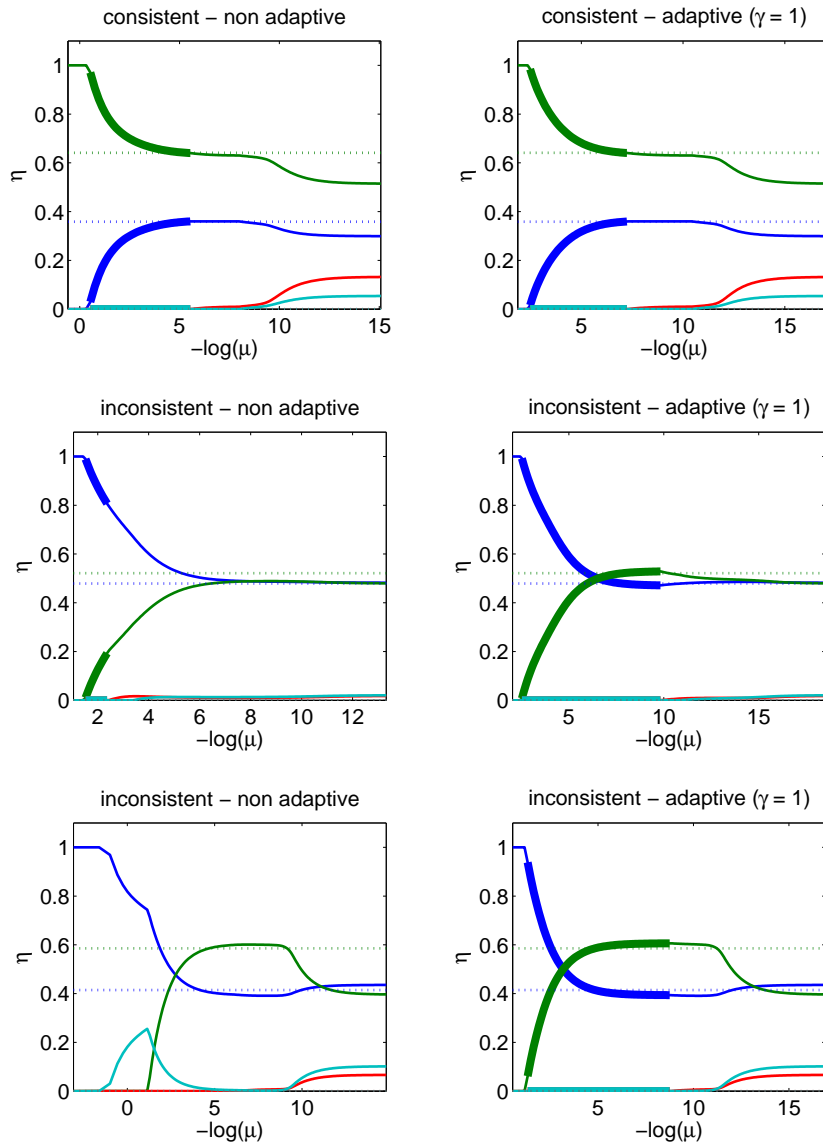


Figure 1: Regularization paths for the group Lasso for two weighting schemes (*left*: non adaptive, *right*: adaptive) and three different population densities (*top*: strict consistency condition satisfied, *middle*: weak condition not satisfied, no model consistent estimates, *bottom*: weak condition not satisfied, some model consistent estimates but without regular consistency). For each of the plots, plain curves correspond to values of estimated $\hat{\eta}_j$, dotted curves to population values η_j , and bold curves to model consistent estimates.

(b) form $\Sigma_{XX} = GG^\top$, (c) for each $j \in \{1, \dots, m\}$, rescale $X_j \in \mathbb{R}^2$ so that $\text{tr}\Sigma_{X_j X_j} = 1$. We selected $\text{Card}(\mathbf{J}) = 2$ groups at random and sampled non zero loading vectors as follows: (a) sample each loading from independent standard normal distributions, (b) rescale those to unit norm, (c) rescale those by a scaling which is uniform at random between $\frac{1}{3}$ and 1. Finally, we chose a constant noise level of standard deviation σ equal to 0.2 times $(\mathbb{E}(w^\top X)^2)^{1/2}$ and sampled Y from a conditional normal distribution with constant variance. The joint distribution on (X, Y) thus defined satisfies with probability one assumptions **(A1-3)**.

For cases when the correlation conditions (4) and (5) were or were not satisfied, we consider two different weighting schemes, i.e., different ways of setting the weights d_j of the block ℓ_1 -norm: unit weights (which correspond to the unit trace weighting scheme) and adaptive weights as defined in Section 4.

In Figure 1, we plot the regularization paths corresponding to 200 i.i.d. samples, computed by the algorithm of Bach et al. (2004b). We only plot the values of the estimated variables $\hat{\eta}_j, j = 1, \dots, m$ for the alternative formulation in Section 2.7, which are proportional to $\|\hat{w}_j\|$ and normalized so that $\sum_{j=1}^m \hat{\eta}_j = 1$. We compare them to the population values η_j : both in terms of values, and in terms of their sparsity pattern (η_j is zero for the weights which are equal to zero). Figure 1 illustrates several of our theoretical results: (a) the top row corresponds to a situation where the strict consistency condition is satisfied and thus we obtain model consistent estimates with also a good estimation of the loading vectors (in the figure, only the good behavior of the norms of these loading vectors are represented); (b) the right column corresponds to the adaptive weighting schemes which also always achieve the two type of consistency; (c) in the middle and bottom rows, the consistency condition was not satisfied, and in the bottom row the condition of Proposition Figure 1 that ensures that we can get model consistent estimates without regular consistency, is met, while it is not in the middle row: as expected, in the bottom row, we get some model consistent estimates but with bad norm estimation.

In Figure 2, 3 and 4, we consider the three joint distributions used in Figure 1 and compute regularization paths for several number of samples (10 to 10^5) with 200 replications. This allows us to estimate both the probability of correct pattern estimation $\mathbb{P}(J(\hat{w}) = \mathbf{J})$ which is considered in Section 2.5, and the logarithm of the expected error $\log \mathbb{E}\|\hat{w} - \mathbf{w}\|^2$.

From Figure 2, it is worth noting (a) the regular spacing between the probability of correct pattern selection for several equally spaced (in log scale) numbers of samples, which corroborates the asymptotic result in Section 2.5. Moreover, (b) in both row, we get model consistent estimates with increasingly smaller norms as the number of samples grow. Finally, (c) the mean square errors are smaller for the adaptive weighting scheme.

From Figure 3, it is worth noting that (a) in the non adaptive case, we have two regimes for the probability of correct pattern selection: a regime corresponding to Proposition 6 where this probability can take values in $[0, 1)$ for increasingly smaller regularization parameters (when n grows); and a regime corresponding to non vanishing limiting regularization parameters corresponding to Proposition 5: we have model consistency without regular consistency. Also, (b) the adaptive weighting scheme allows both consistencies. In Figure 3 however, the second regime (correct model estimates, inconsistent estimation of loadings) is not present.

In Figure 5, we sampled 10,000 different covariance matrices and loading vectors using the procedure described above. For each of these we computed the regularization paths from 1000 samples, and we classify each path into three categories: (1) existence of model consistent estimates with estimation error $\|\hat{w} - \mathbf{w}\|$ less than 10^{-1} , (2) existence of model consistent estimates but none

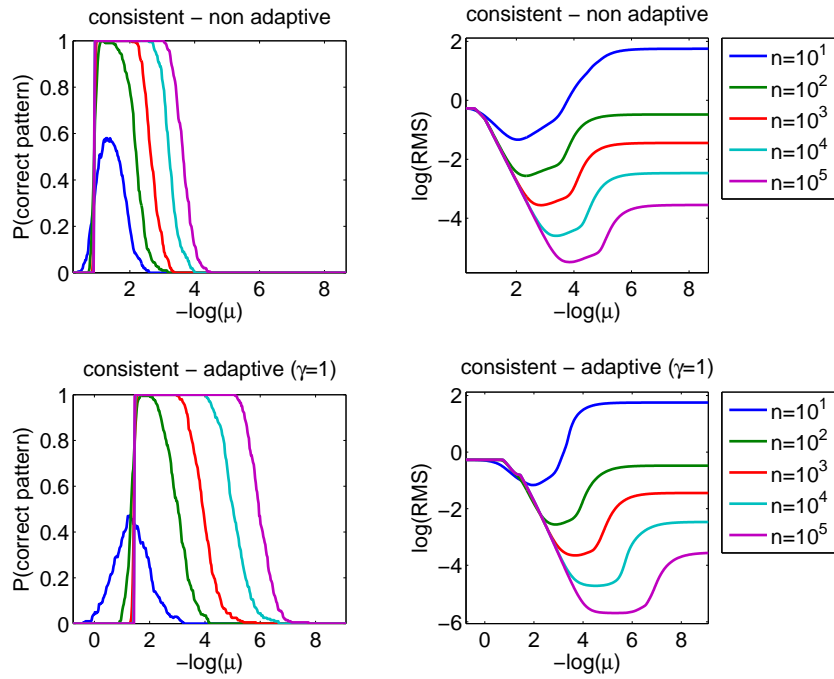


Figure 2: Synthetic example where consistency condition in Eq. (4) is satisfied (same example as the top of Figure 1: probability of correct pattern selection (*left*) and logarithm of the expected mean squared estimation error (*right*), for several number of samples as a function of the regularization parameter, for regular regularization (*top*), adaptive regularization with $\gamma = 1$ (*bottom*).

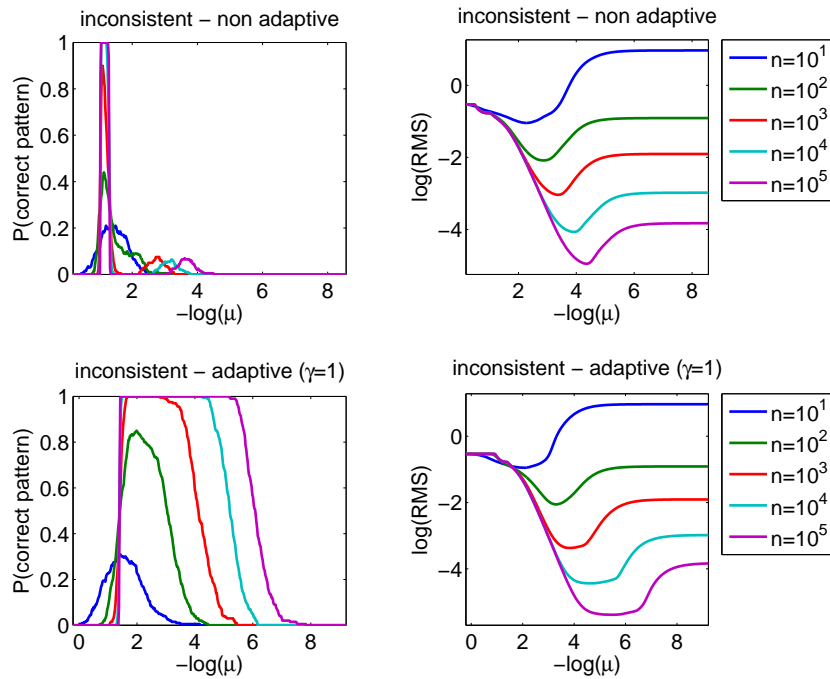


Figure 3: Synthetic example where consistency condition in Eq. (5) is not satisfied (same example as the middle of Figure 1: probability of correct pattern selection (*left*) and logarithm of the expected mean squared estimation error (*right*), for several number of samples as a function of the regularization parameter, for regular regularization (*top*), adaptive regularization with $\gamma = 1$ (*bottom*).

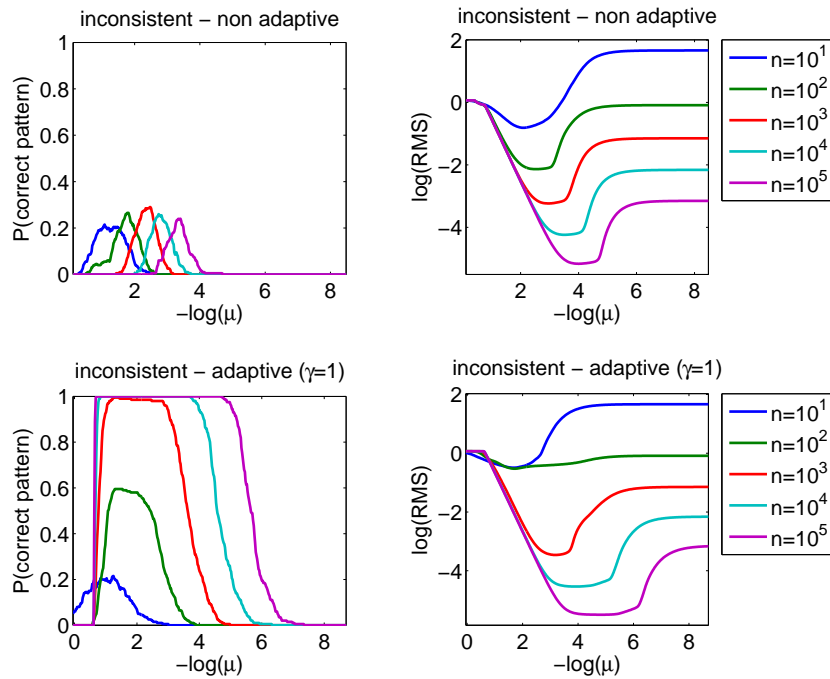


Figure 4: Synthetic example where consistency condition in Eq. (5) is not satisfied (same example as the bottom of Figure 1: probability of correct pattern selection (*left*) and logarithm of the expected mean squared estimation error (*right*), for several number of samples as a function of the regularization parameter, for regular regularization (*top*), adaptive regularization with $\gamma = 1$ (*bottom*).

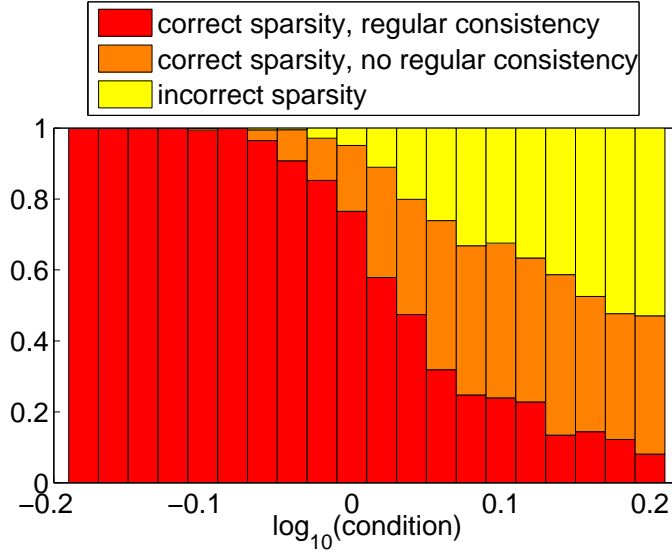


Figure 5: Consistency of estimation vs. consistency condition. See text for details.

with estimation error $\|\hat{w} - \mathbf{w}\|$ less than 10^{-1} and (3) non existence of model consistent estimates. In Figure 5 we plot the proportion of each of the three class as a function of the logarithm of $\max_{i \in \mathcal{J}^c} \frac{1}{d_i} \left\| \Sigma_{X_i X_{\mathcal{J}}} \Sigma_{X_{\mathcal{J}} X_{\mathcal{J}}}^{-1} \text{Diag}(d_j / \|\mathbf{w}_j\|) \mathbf{w}_{\mathcal{J}} \right\|$. The position of the previous value with respect to 1 is indicative of the expected model consistency. When it is less than one, then we get with overwhelming probability model consistent estimates with good errors. As the condition gets larger than one, we get fewer such good estimates and more and more model inconsistent estimates.

5.2 Nonparametric Case

In the infinite dimensional group case, we sampled $X \in \mathbb{R}^m$ from a normal distribution with zero mean vector and a covariance matrix of size $m = 4$, generated as follows: (a) sample a $m \times m$ matrix G with independent standard normal distributions, (b) form $\Sigma_{XX} = GG^{\top}$, (c) for each $j \in \{1, \dots, m\}$, rescale $X_j \in \mathbb{R}$ so that $\Sigma_{X_j X_j} = 1$.

We use the same Gaussian kernel for each variables, $k(x, x') = e^{-(x-x')^2}$. In this situation, as shown in Appendix E we can compute in closed form the eigenfunctions and eigenvalues of the marginal covariance operators. We then sample function from random independent components on the first 10 eigenfunctions. Examples are given in Figure 6.

In Figure 7, we plot the regularization paths corresponding to 1000 i.i.d. samples, computed by the algorithm of Bach et al. (2004b). We only plot the values of the estimated variables $\hat{\eta}_j, j = 1, \dots, m$ for the alternative formulation in Section 2.7, which are proportional to $\|\hat{w}_j\|$ and normalized so that $\sum_{j=1}^m \hat{\eta}_j = 1$. We compare them to the population values η_j : both in terms of values, and in terms of their sparsity pattern (η_j is zero for the weights which are equal to zero). Figure 7 illustrates several of our theoretical results: (a) the top row corresponds to a situation where the strict consistency condition is satisfied and thus we obtain model consistent estimates with also a good estimation of the loading vectors (in the figure, only the good behavior of the norms of these

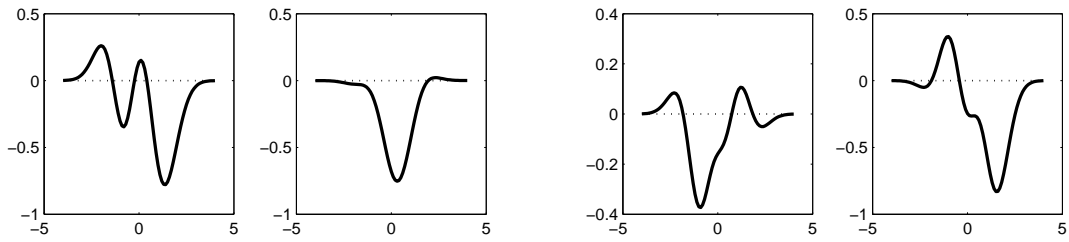


Figure 6: Functions to be estimated in the synthetic non parametric group Lasso experiments (left: consistent case, right: inconsistent case).

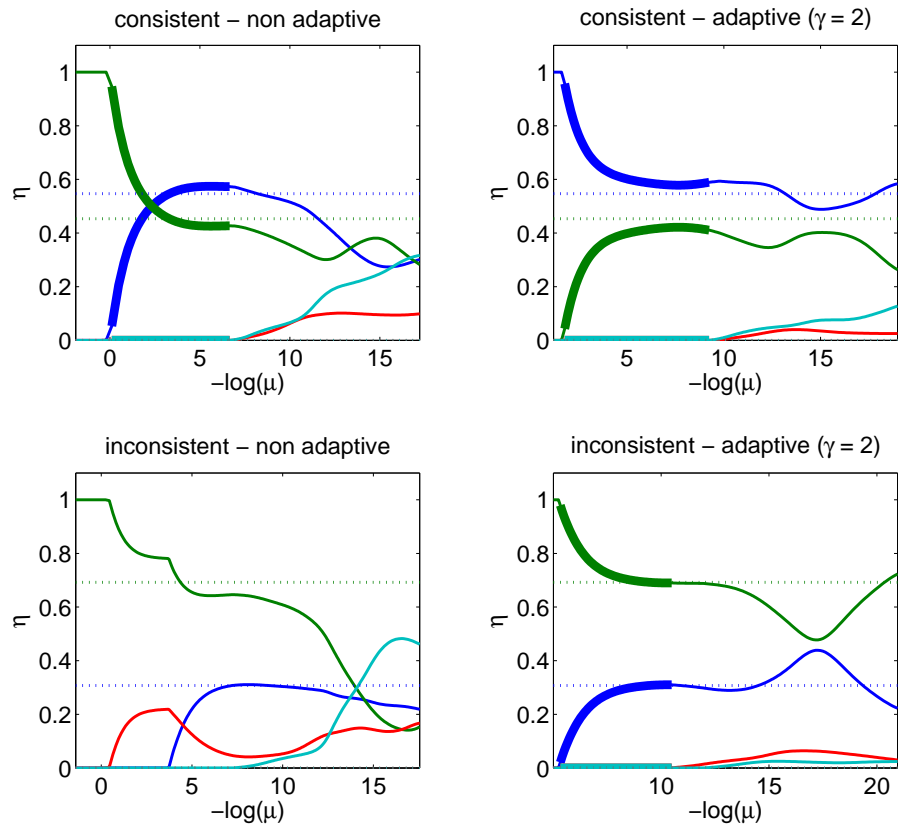


Figure 7: Regularization paths for the group Lasso for two weighting schemes (*left*: non adaptive, *right*: adaptive) and two different population densities (*top*: strict consistency condition satisfied, *bottom*: weak condition not satisfied). For each of the plots, plain curves correspond to values of estimated $\hat{\eta}_j$, dotted curves to population values η_j , and bold curves to model consistent estimates.

loading vectors are represented); (b) in the bottom row, the consistency condition was not satisfied, and we do not get good model estimates. Finally, (b) the right column corresponds to the adaptive weighting schemes which also always achieve the two type of consistency. However, such schemes should be used with care, as there is one added free parameter (the regularization parameter κ of the least-square estimate used to define the weights): if chosen too large, all adaptive weights are equal, and thus there is no adaptation, while if chosen too small, the least-square estimate may overfit.

6. Conclusion

In this paper, we have extended some of the theoretical results of the Lasso to the group Lasso, for finite dimensional groups and infinite dimensional groups. In particular, under practical assumptions regarding the distributions the data are sampled from, we have provided necessary and sufficient conditions for model consistency of the group Lasso and its nonparametric version, multiple kernel learning.

The current work could be extended in several ways: first, a more detailed study of the limiting distributions of the group Lasso and adaptive group Lasso estimators could be carried and then extend the analysis of Zou (2006) or Juditsky and Nemirovski (2000) and Wu et al. (2007), in particular regarding convergence rates. Second, our results should extend to generalized linear models, such as logistic regression (Meier et al., 2006). Also, it is of interest to let the number m of groups or kernels to grow unbounded and extend the results of Zhao and Yu (2006) and Meinshausen and Yu (2006) to the group Lasso. Finally, similar analysis may be carried through for more general norms with different sparsity inducing properties (Bach, 2007).

Appendix A. Proof of Optimization Results

In this appendix, we give detailed proofs of the various propositions on optimality conditions and dual problems.

A.1 Proof of Proposition 1

We rewrite problem in Eq. (1), in the form

$$\min_{w \in \mathbb{R}^p, v \in \mathbb{R}^m} \frac{1}{2} \hat{\Sigma}_{YY} - \hat{\Sigma}_{YX} w + \frac{1}{2} w^\top \hat{\Sigma}_{XX} w + \lambda_n \sum_{j=1}^m d_j v_j,$$

with added constraints that $\forall j, \|w_j\| \leq v_j$. In order to deal with these constraints we use the tools from conic programming with the second-order cone, also known as the ‘‘ice cream’’ cone (Boyd and Vandenberghe, 2003). We consider the Lagrangian with dual variables $(\beta_j, \gamma_j) \in \mathbb{R}^{p_j} \times \mathbb{R}$ such that $\|\beta_j\| \leq \gamma_j$:

$$\mathcal{L}(w, v, \beta, \gamma) = \frac{1}{2} \hat{\Sigma}_{YY} - \hat{\Sigma}_{YX} w + \frac{1}{2} w^\top \hat{\Sigma}_{XX} w + \lambda_n d^\top v - \sum_{j=1}^m \begin{pmatrix} w_j \\ v_j \end{pmatrix}^\top \begin{pmatrix} \beta_j \\ \gamma_j \end{pmatrix}.$$

The derivatives with respect to primal variables are

$$\begin{aligned}\nabla_w \mathcal{L}(w, v, \beta, \gamma) &= \hat{\Sigma}_{XX} w - \hat{\Sigma}_{XY} - \beta, \\ \nabla_v \mathcal{L}(w, v, \beta, \gamma) &= \lambda_n d - \gamma.\end{aligned}$$

At optimality, primal and dual variables are completely characterized by w and β . Since the dual and the primal problems are strictly feasible, strong duality holds and the KKT conditions for reduced primal/dual variables (w, β) are

$$\forall j, \|\beta_j\| \leq \lambda_n d_j \quad (\text{dual feasibility}) , \quad (24)$$

$$\forall j, \beta_j = \hat{\Sigma}_{X_j X} w - \hat{\Sigma}_{X_j Y} \quad (\text{stationarity}) , \quad (25)$$

$$\forall j, \beta_j^\top w_j + \|w_j\| \lambda_n d_j = 0 \quad (\text{complementary slackness}) . \quad (26)$$

Complementary slackness for the second order cone has special consequences: $w_j^\top \beta_j + \|w_j\| \lambda_n d_j = 0$ if and only if (Boyd and Vandenberghe, 2003, Lobo et al., 1998), either (a) $w_j = 0$, or (b) $w_j \neq 0$, $\|\beta_j\| = \lambda_n d_j$ and $\exists \eta_j > 0$ such that $w_j = -\frac{\eta_j}{\lambda_n} \beta_j$ (anti-proportionality), which implies $\beta_j = -w_j \frac{\lambda_n d_j}{\|w_j\|}$ and $\eta_j = \|w_j\|/d_j$. This leads to the proposition.

A.2 Proof of Proposition 8

We follow the proof of Proposition 1 and of Bach et al. (2004a). We rewrite problem in Eq. (12), in the form

$$\min_{w \in \mathbb{R}^p, v \in \mathbb{R}^m, t \in \mathbb{R}} \frac{1}{2} \hat{\Sigma}_{YY} - \hat{\Sigma}_{YX} w + \frac{1}{2} w^\top \hat{\Sigma}_{XX} w + \frac{1}{2} \mu_n t^2,$$

with constraints that $\forall j, \|w_j\| \leq v_j$ and $d^\top v \leq t$. We consider the Lagrangian with dual variables $(\beta_j, \gamma_j) \in \mathbb{R}^{p_j} \times \mathbb{R}$ and $\delta \in \mathbb{R}_+$ such that $\|\beta_j\| \leq \gamma_j, j = 1, \dots, m$:

$$\mathcal{L}(w, v, \beta, \gamma, \delta) = \frac{1}{2} \hat{\Sigma}_{YY} - \hat{\Sigma}_{YX} w + \frac{1}{2} w^\top \hat{\Sigma}_{XX} w + \frac{1}{2} \mu_n t^2 - \beta^\top w - \gamma^\top v + \delta(d^\top v - t).$$

The derivatives with respect to primal variables are

$$\begin{aligned}\nabla_w \mathcal{L}(w, v, \beta, \gamma) &= \hat{\Sigma}_{XX} w - \hat{\Sigma}_{XY} - \beta, \\ \nabla_v \mathcal{L}(w, v, \beta, \gamma) &= \delta d - \gamma, \\ \nabla_t \mathcal{L}(w, v, \beta, \gamma) &= \mu_n t - \delta.\end{aligned}$$

At optimality, primal and dual variables are completely characterized by w and β . Since the dual and the primal problems are strictly feasible, strong duality holds and the KKT conditions for reduced primal/dual variables (w, β) are

$$\forall j, \beta_j = \hat{\Sigma}_{X_j X} w - \hat{\Sigma}_{X_j Y} \quad (\text{stationarity - 1}) , \quad (27)$$

$$\forall j, \sum_{j=1}^m d_j \|w_j\| = \frac{1}{\mu_n} \max_{i=1, \dots, m} \frac{\|\beta_i\|}{d_i} \quad (\text{stationarity - 2}) , \quad (28)$$

$$\forall j, \left(\frac{\beta_j}{d_j} \right)^\top w_j + \|w_j\| \max_{i=1, \dots, m} \frac{\|\beta_i\|}{d_i} = 0 \quad (\text{complementary slackness}) . \quad (29)$$

Complementary slackness for the second order cone implies that:

$$\left(\frac{\beta_j}{d_j}\right)^\top w_j + \|w_j\| \max_{i=1,\dots,m} \frac{\|\beta_i\|}{d_i} = 0,$$

if and only if, either (a) $w_j = 0$, or (b) $w_j \neq 0$ and $\frac{\|\beta_j\|}{d_j} = \max_{i=1,\dots,m} \frac{\|\beta_i\|}{d_i}$, and $\exists \eta_j \geq 0$ such that $w_j = -\eta_j \beta_j / \mu_n$, which implies $\|w_j\| = \frac{\eta_j d_j}{\mu_n} \max_{i=1,\dots,m} \frac{\|\beta_i\|}{d_i}$.

By writing $\eta_j = 0$ if $w_j = 0$ (i.e., in order to cover all cases), we have from Eq. (28) $\sum_{j=1}^m d_j \|w_j\| = \frac{1}{\mu_n} \max_{i=1,\dots,m} \frac{\|\beta_i\|}{d_i}$, which implies $\sum_{j=1}^m d_j^2 \eta_j = 1$ and thus $\forall j, \eta_j = \frac{\|w_j\|/d_j}{\sum_i d_i \|w_i\|}$. This leads to $\forall j, \beta_j = -w_j \mu_n / \eta_j = -\frac{w_j}{\|w_j\|} \sum_{i=1}^n d_i \|w_i\|$. The proposition follows.

A.3 Proof of Proposition 10

By following the usual proof of the representer theorem (Wahba, 1990), we obtain that each optimal function f_j must be supported by the data points, i.e., there exists $\alpha = (\alpha_1, \dots, \alpha_m) \in \mathbb{R}^{n \times m}$ such that for all $j = 1, \dots, m$, $f_j = \sum_{i=1}^n \alpha_{ij} k_j(\cdot, x_{ij})$. When using this representation back into Eq. (15), we obtain an optimization problem that only depends on $\phi_j = G_j^\top \alpha_j$ for $j = 1, \dots, m$ where G_j denotes any square root of the kernel matrix K_j , i.e., $K_j = G_j G_j^\top$. This problem is exactly the finite dimensional problem in Eq. (12), where \bar{X}_j is replaced by G_j and w_j by ϕ_j . Thus Proposition 8 applies and we can easily derive the current proposition by expressing all terms through the functions f_j . Note that in this proposition, we do not show that the $\alpha_j, j = 1, \dots, m$, are all proportional to the same vector, as is done in Appendix A.4.

A.4 Proof of Proposition 13

We prove the proposition in the linear case. Going to the general case, can be done in the same way as done in Appendix A.3. We let \bar{X} denote the covariate matrix in $\mathbb{R}^{n \times p}$; we simply need to add a new variable $u = \bar{X}w + b1_n$ and to “dualize” it. That is, we rewrite problem in Eq. (12), in the form

$$\min_{w \in \mathbb{R}^p, b \in \mathbb{R}, v \in \mathbb{R}^m, t \in \mathbb{R}, u \in \mathbb{R}^n} \frac{1}{2n} \|\bar{Y} - u\|^2 + \frac{1}{2} \mu_n t^2,$$

with constraints that $\forall j, \|w_j\| \leq v_j, d^\top v \leq t$ and $\bar{X}w + b1_n = u$. We consider the Lagrangian with dual variables $(\beta_j, \gamma_j) \in \mathbb{R}^{p_j} \times \mathbb{R}$ and $\delta \in \mathbb{R}_+$ such that $\|\beta_j\| \leq \gamma_j$, and $\alpha \in \mathbb{R}^n$:

$$\mathcal{L}(w, b, v, u, \beta, \gamma, \alpha, \delta) = \frac{1}{2n} \|\bar{Y} - u\|^2 + \mu_n \alpha^\top (u - \bar{X}w) + \frac{1}{2} \mu_n t^2 - \sum_{j=1}^m \left\{ \beta_j^\top w_j + \gamma_j v_j \right\} + \delta (d^\top v - t).$$

The derivatives with respect to primal variables are

$$\begin{aligned} \nabla_w \mathcal{L}(w, v, u, \beta, \gamma, \alpha) &= -\mu_n \bar{X}^\top \alpha - \beta \\ \nabla_v \mathcal{L}(w, v, u, \beta, \gamma, \alpha) &= \delta d - \gamma \\ \nabla_t \mathcal{L}(w, v, u, \beta, \gamma, \alpha) &= \mu_n t - \delta \\ \nabla_u \mathcal{L}(w, v, u, \beta, \gamma, \alpha) &= \frac{1}{n} (u - \bar{Y} + \mu_n n \alpha) \\ \nabla_b \mathcal{L}(w, v, u, \beta, \gamma, \alpha) &= \mu_n \alpha^\top 1_n. \end{aligned}$$

Equating them to zero, we get the dual problem in Eq. (20). Since the dual and the primal problems are strictly feasible, strong duality holds and the KKT conditions for reduced primal/dual variables (w, α) are

$$\forall j, \bar{X}w - \bar{Y} + \mu_n n \alpha = 0 \quad (\text{stationarity - 1}), \quad (30)$$

$$\forall j, \sum_{i=1}^m d_j \|w_j\| = \max_{i=1, \dots, m} \frac{(\alpha^\top K_i \alpha)^{1/2}}{d_i} \quad (\text{stationarity - 2}), \quad (31)$$

$$\alpha^\top 1_n = 0 \quad (\text{stationarity - 3}), \quad (32)$$

$$\forall j, \left(\frac{-\bar{X}_j^\top \alpha}{d_j} \right)^\top w_j + \|w_j\| \max_{i=1, \dots, m} \frac{(\alpha^\top K_i \alpha)^{1/2}}{d_i} = 0 \quad (\text{complementary slackness}). \quad (33)$$

Complementary slackness for the second order cone goes leads to:

$$\left(\frac{-\bar{X}_j^\top \alpha}{d_j} \right)^\top w_j + \|w_j\| \max_{i=1, \dots, m} \frac{(\alpha^\top K_i \alpha)^{1/2}}{d_i} = 0,$$

if and only if, either (a) $w_j = 0$, or (b) $w_j \neq 0$ and $\frac{(\alpha^\top K_j \alpha)^{1/2}}{d_j} = \max_{i=1, \dots, m} \frac{(\alpha^\top K_i \alpha)^{1/2}}{d_i}$, and $\exists \eta_j \geq 0$

such that $w_j = -\eta_j \left(-\bar{X}_j^\top \alpha \right)$, which implies $\|w_j\| = \eta_j d_j \max_{i=1, \dots, m} \frac{(\alpha^\top K_i \alpha)^{1/2}}{d_i}$.

By writing $\eta_j = 0$ if $w_j = 0$ (to cover all cases), we have from Eq. (31), $\sum_{j=1}^m d_j \|w_j\| = \max_{i=1, \dots, m} \frac{(\alpha^\top K_i \alpha)^{1/2}}{d_i}$, which implies $\sum_{j=1}^m d_j^2 \eta_j = 1$. The proposition follows from the fact that at optimality, $\forall j, w_j = \eta_j \bar{X}_j^\top \alpha$.

A.5 Proof of Proposition 14

What makes this proposition non obvious is the fact that the covariance operator Σ_{XX} is not invertible in general. From proposition 13, we know that each f_j must be of the form $f_j = \eta_j \sum_{i=1}^n \alpha_i k_j(x_{ij}, \cdot)$, where α is *uniquely* defined. Moreover, η is such that $\left(\sum_{j=1}^m \eta_j K_j + n \mu_n I_n \right) \alpha = \bar{Y}$ and such that if $\frac{\alpha^\top K_j \alpha}{d_j^2} < A$, then $\eta_j = 0$ (where $A = \max_{i=1, \dots, m} \frac{\alpha^\top K_i \alpha}{d_i^2}$). Thus, if the solution is not unique, there exists two vectors $\eta \neq \zeta$ such that η and ζ have zero components on indices j such that $\alpha^\top K_j \alpha < A d_j^2$ (we let denote J the active set and thus J^c this set of indices), and $\sum_{j=1}^m (\zeta_j - \eta_j) K_j \alpha = 0$. This implies that the vectors $\Pi_n K_j \alpha = \Pi_n K_j \Pi_n \alpha$, $j \in J$ are linearly dependent. Those vectors are exactly the centered vector of values of the functions $g_j = \sum_{i=1}^n \alpha_i k_j(x_{ij}, \cdot)$ at the observed data points. Thus, non unicity implies that the empirical covariance matrix of the random variables $g_j(X_j)$, $j \in J$, is non invertible. Moreover, we have $\|g_j\|_{\mathcal{F}_j}^2 = \alpha^\top K_j \alpha = d_j^2 A > 0$ and the empirical marginal variance of $g_j(X_j)$ is equal to $\alpha^\top K_j^2 \alpha > 0$ (otherwise $\|g_j\|_{\mathcal{F}_j}^2 = 0$). By normalizing by the (non vanishing) empirical standard deviations, we thus obtain functions such that the empirical covariance matrix is singular, but the marginal empirical variance are equal to one. Because the empirical covariance operator is a consistent estimator of Σ_{XX} and C_{XX} is invertible, we get a contradiction, which proves the unicity of solutions.

Appendix B. Detailed Proofs for the Group Lasso

In this appendix, detailed proofs of the consistency results for the finite dimensional case (Theorems 2 and 3) are presented. Some of the results presented in this appendix are corollaries of the more general results in Appendix C, but their proofs in the finite dimensional case are much simpler.

B.1 Proof of Theorem 2

We begin with a lemma, which states that if we restrict ourselves to the covariates which we are after (i.e., indexed by \mathbf{J}), we get a consistent estimate as soon as λ_n tends to zero:

Lemma 20 *Assume (A1-3). Let $\tilde{w}_{\mathbf{J}}$ any minimizer of*

$$\frac{1}{2n} \|\bar{Y} - \bar{X}_{\mathbf{J}} w_{\mathbf{J}}\|^2 + \lambda_n \sum_{j \in \mathbf{J}} d_j \|w_j\| = \frac{1}{2} \hat{\Sigma}_{Y Y} - \hat{\Sigma}_{Y X_{\mathbf{J}}} w_{\mathbf{J}} + \frac{1}{2} w_{\mathbf{J}}^{\top} \hat{\Sigma}_{X_{\mathbf{J}} X_{\mathbf{J}}} w_{\mathbf{J}} + \lambda_n \sum_{j \in \mathbf{J}} d_j \|w_j\|.$$

If $\lambda_n \rightarrow 0$, then $\tilde{w}_{\mathbf{J}}$ converges to $w_{\mathbf{J}}$ in probability.

Proof If λ_n tends to zero, then the cost function defining $\tilde{w}_{\mathbf{J}}$ converges to $F_n(w_{\mathbf{J}}) = \frac{1}{2} \Sigma_{Y Y} - \Sigma_{Y X_{\mathbf{J}}} w_{\mathbf{J}} + \frac{1}{2} w_{\mathbf{J}}^{\top} \Sigma_{X_{\mathbf{J}} X_{\mathbf{J}}} w_{\mathbf{J}}$ whose unique (because $\Sigma_{X_{\mathbf{J}} X_{\mathbf{J}}}$ is positive definite) global minimum is $w_{\mathbf{J}}$ (true generating value). The convergence of $\tilde{w}_{\mathbf{J}}$ is thus a simple consequence of standard results in M -estimation (Van der Vaart, 1998, Fu and Knight, 2000). \blacksquare

We now prove Theorem 2. Let $\tilde{w}_{\mathbf{J}}$ be defined as in Lemma 20. We extend it by zeros on \mathbf{J}^c . We already know from Lemma 20 that we have consistency in squared norm. Since with probability tending to one, the problem has a unique solution (because $\Sigma_{X X}$ is invertible), we now need to prove that the probability that \tilde{w} is optimal for problem in Eq. (1) is tending to one.

By definition of $\tilde{w}_{\mathbf{J}}$, the optimality condition (3) is satisfied. We now need to verify optimality condition (2). Denoting $\varepsilon = Y - \mathbf{w}^{\top} X - \mathbf{b}$, we have:

$$\hat{\Sigma}_{X Y} = \hat{\Sigma}_{X X} \mathbf{w} + \hat{\Sigma}_{X \varepsilon} = \left(\Sigma_{X X} + O_p(n^{-1/2}) \right) \mathbf{w} + O_p(n^{-1/2}) = \Sigma_{X X_{\mathbf{J}}} \mathbf{w}_{\mathbf{J}} + O_p(n^{-1/2}),$$

because of classical results on convergence of empirical covariances to covariances (Van der Vaart, 1998), which are applicable because we have the fourth order moment condition (A1). We thus have:

$$\hat{\Sigma}_{X Y} - \hat{\Sigma}_{X X_{\mathbf{J}}} \tilde{w}_{\mathbf{J}} = \Sigma_{X X_{\mathbf{J}}} (\mathbf{w}_{\mathbf{J}} - \tilde{w}_{\mathbf{J}}) + O_p(n^{-1/2}). \quad (34)$$

From the optimality condition $\hat{\Sigma}_{X_{\mathbf{J}} Y} - \hat{\Sigma}_{X_{\mathbf{J}} X_{\mathbf{J}}} \tilde{w}_{\mathbf{J}} = \lambda_n \text{Diag}(d_j / \|\tilde{w}_j\|) \tilde{w}_{\mathbf{J}}$ defining $\tilde{w}_{\mathbf{J}}$ and Eq. (34), we obtain:

$$\tilde{w}_{\mathbf{J}} - \mathbf{w}_{\mathbf{J}} = -\lambda_n \Sigma_{X_{\mathbf{J}} X_{\mathbf{J}}}^{-1} \text{Diag}(d_j / \|\tilde{w}_j\|) \tilde{w}_{\mathbf{J}} + O_p(n^{-1/2}). \quad (35)$$

Therefore,

$$\begin{aligned} \hat{\Sigma}_{X_{\mathbf{J}^c} Y} - \hat{\Sigma}_{X_{\mathbf{J}^c} X_{\mathbf{J}}} \tilde{w}_{\mathbf{J}} &= \Sigma_{X_{\mathbf{J}^c} X_{\mathbf{J}}} (\mathbf{w}_{\mathbf{J}} - \tilde{w}_{\mathbf{J}}) + O_p(n^{-1/2}) \text{ by Eq. (34) ,} \\ &= \lambda_n \Sigma_{X_{\mathbf{J}^c} X_{\mathbf{J}}} \Sigma_{X_{\mathbf{J}} X_{\mathbf{J}}}^{-1} \text{Diag}(d_j / \|\tilde{w}_j\|) \tilde{w}_{\mathbf{J}} + O_p(n^{-1/2}) \text{ by Eq. (35).} \end{aligned}$$

Since \tilde{w} is consistent, and $\lambda_n n^{1/2} \rightarrow +\infty$, then for each $i \in \mathbf{J}^c$,

$$\frac{1}{d_i \lambda_n} \left(\hat{\Sigma}_{X_i Y} - \hat{\Sigma}_{X_i X_{\mathbf{J}}} \tilde{w}_{\mathbf{J}} \right)$$

converges in probability to $\frac{1}{d_i} \Sigma_{X_i X_J} \Sigma_{X_J X_J}^{-1} \text{Diag}(d_j / \|\mathbf{w}_j\|) \mathbf{w}_J$ which is of norm *strictly* smaller than one because condition (4) is satisfied. Thus the probability that \tilde{w} is indeed optimal, which is equal to

$$\mathbb{P} \left\{ \forall i \in \mathbf{J}^c, \frac{1}{d_i \lambda_n} \left\| \hat{\Sigma}_{X_i Y} - \hat{\Sigma}_{X_i X_J} \tilde{w}_J \right\| \leq 1 \right\} \geq \prod_{i \in \mathbf{J}^c} \mathbb{P} \left\{ \frac{1}{d_i \lambda_n} \left\| \hat{\Sigma}_{X_i Y} - \hat{\Sigma}_{X_i X_J} \tilde{w}_J \right\| \leq 1 \right\},$$

is tending to 1, which implies the theorem.

B.2 Proof of Theorem 3

We prove the theorem by contradiction, by assuming that there exists $i \in \mathbf{J}^c$ such that

$$\frac{1}{d_i} \left\| \Sigma_{X_i X_J} \Sigma_{X_J X_J}^{-1} \text{Diag}(d_j / \|\mathbf{w}_j\|) \mathbf{w}_J \right\| > 1.$$

Since with probability tending to one $J(\hat{w}) = \mathbf{J}$, with probability tending to one, we have from optimality condition (3):

$$\hat{w}_J = \hat{\Sigma}_{X_J X_J}^{-1} \left(\hat{\Sigma}_{X_J Y} - \lambda_n \text{Diag}(d_j / \|\hat{w}_j\|) \hat{w}_J \right),$$

and thus

$$\begin{aligned} \hat{\Sigma}_{X_i Y} - \hat{\Sigma}_{X_i X_J} \hat{w}_J &= (\hat{\Sigma}_{X_i Y} - \hat{\Sigma}_{X_i X_J} \hat{\Sigma}_{X_J X_J}^{-1} \hat{\Sigma}_{X_J Y}) + \lambda_n \hat{\Sigma}_{X_i X_J} \hat{\Sigma}_{X_J X_J}^{-1} \text{Diag}(d_j / \|\hat{w}_j\|) \hat{w}_J \\ &= A_n + B_n. \end{aligned}$$

The second term B_n in the last expression (divided by λ_n) converges to

$$v = \Sigma_{X_i X_J} \Sigma_{X_J X_J}^{-1} \text{Diag}(d_j / \|\mathbf{w}_j\|) \mathbf{w}_J \in \mathbb{R}^{p_j},$$

because \hat{w} is assumed to converge in probability to \mathbf{w} and empirical covariance matrices converge to population covariance matrices. By assumption $\|v\| > d_i$, which implies that the probability $\mathbb{P} \left\{ \left(\frac{v}{\|v\|} \right)^\top (B_n / \lambda_n) \geq (d_i + \|v\|) / 2 \right\}$ converges to one.

The first term is equal to (with $\varepsilon_k = y_k - \mathbf{w}^\top x_k - \mathbf{b}_k$ and $\text{epsilon} = \frac{1}{n} \sum_{k=1}^n \varepsilon_k$):

$$\begin{aligned} A_n &= \hat{\Sigma}_{X_i Y} - \hat{\Sigma}_{X_i X_J} \hat{\Sigma}_{X_J X_J}^{-1} \hat{\Sigma}_{X_J Y} \\ &= \hat{\Sigma}_{X_i X_J} \mathbf{w}_J - \hat{\Sigma}_{X_i X_J} \hat{\Sigma}_{X_J X_J}^{-1} \hat{\Sigma}_{X_J X_J} \mathbf{w}_J + \hat{\Sigma}_{X_i \varepsilon} - \hat{\Sigma}_{X_i X_J} \hat{\Sigma}_{X_J X_J}^{-1} \hat{\Sigma}_{X_J \varepsilon} \\ &= \hat{\Sigma}_{X_i \varepsilon} - \hat{\Sigma}_{X_i X_J} \hat{\Sigma}_{X_J X_J}^{-1} \hat{\Sigma}_{X_J \varepsilon} \\ &= \hat{\Sigma}_{X_i \varepsilon} - \Sigma_{X_i X_J} \Sigma_{X_J X_J}^{-1} \hat{\Sigma}_{X_J \varepsilon} + o_p(n^{-1/2}) \\ &= \frac{1}{n} \sum_{k=1}^n (\varepsilon_k - \bar{\varepsilon}) \left(x_{ki} - \Sigma_{X_i X_J} \Sigma_{X_J X_J}^{-1} x_{kJ} \right) + o_p(n^{-1/2}) = C_n + o_p(n^{-1/2}). \end{aligned}$$

The random variable C_n is a U-statistic with square integrable kernel obtained from i.i.d. random vectors; it is thus asymptotically normal (Van der Vaart, 1998). We thus simply need to

compute the mean and the variance of C_n . We have $\mathbb{E}C_n = 0$ because $\mathbb{E}(X\varepsilon) = \Sigma_{X\varepsilon} = 0$. We let denote $D_k = x_{ki} - \Sigma_{X_i X_J} \Sigma_{X_J X_J}^{-1} x_{kJ} - \frac{1}{n} \sum_{k=1}^n x_{ki} - \Sigma_{X_i X_J} \Sigma_{X_J X_J}^{-1} x_{kJ}$. We have:

$$\begin{aligned}
\text{var}(C_n) &= \mathbb{E}C_n^2 = \mathbb{E}(\mathbb{E}(C_n^2|\bar{X})) \\
&= \mathbb{E} \left[\frac{1}{n^2} \sum_{k=1}^n E(\varepsilon_k^2|\bar{X}) D_k D_k^\top \right] \\
&\succcurlyeq \mathbb{E} \left[\frac{1}{n^2} \sum_{k=1}^n \sigma_{\min}^2 D_k D_k^\top \right] \\
&= \frac{1}{n} \sigma_{\min}^2 \mathbb{E} \left(\hat{\Sigma}_{X_i X_i} - \Sigma_{X_i X_J} \Sigma_{X_J X_J}^{-1} \hat{\Sigma}_{X_J X_i} \right) \\
&= \frac{n-1}{n^2} \sigma_{\min}^2 \left(\Sigma_{X_i X_i} - \Sigma_{X_i X_J} \Sigma_{X_J X_J}^{-1} \Sigma_{X_J X_i} \right),
\end{aligned}$$

where $M \succcurlyeq N$ denotes the partial order between symmetric matrices (i.e., equivalent to $M - N$ positive semidefinite).

Thus $n^{1/2}C_n$ is asymptotically normal with mean 0 and covariance matrix larger than $\sigma_{\min}^2 \Sigma_{X_i|X_J} = \sigma_{\min}^2 \times (\Sigma_{X_i X_i} - \Sigma_{X_i X_J} \Sigma_{X_J X_J}^{-1} \Sigma_{X_J X_i})$ which is positive definite (because this is the conditional covariance of X_i given X_J and Σ_{XX} is assumed invertible). Therefore $\mathbb{P}(n^{1/2}v^\top A_n > 0)$ converges to a constant $a \in (0, 1)$, which implies that $\mathbb{P} \left\{ \frac{v}{\|v\|}^\top (A_n + B_n) / \lambda_n \geq (d_i + \|v\|) / 2 \right\}$ is asymptotically bounded below by a . Thus, since $\|(A_n + B_n) / \lambda_n\| \geq \frac{v}{\|v\|}^\top (A_n + B_n) / \lambda_n \geq (d_i + \|v\|) / 2 > d_i$ implies that \hat{w} is not optimal, we get a contradiction, which concludes the proof.

B.3 Proof of Theorem 4

We first prove the following refinement of Lemma 20:

Lemma 21 *Assume (A1-3). Let \tilde{w}_J any minimizer of*

$$\frac{1}{2n} \|\bar{Y} - \bar{X}_J w_J\|^2 + \lambda_n \sum_{j \in J} d_j \|w_j\| = \frac{1}{2} \hat{\Sigma}_{Y Y} - \hat{\Sigma}_{Y X_J} w_J + \frac{1}{2} w_J^\top \hat{\Sigma}_{X_J X_J} w_J + \lambda_n \sum_{j \in J} d_j \|w_j\|.$$

If $\lambda_n \rightarrow 0$ and $\lambda_n n^{1/2} \rightarrow \infty$, then $\frac{1}{\lambda_n}(\tilde{w}_J - w_J)$ converges in probability to

$$\Delta = -\Sigma_{X_J X_J}^{-1} \text{Diag}(d_j / \|w_j\|) w_J.$$

Proof We follow Fu and Knight (2000) and write $\tilde{w}_J = w_J + \lambda_n \tilde{\Delta}$. The vector $\tilde{\Delta}$ is the minimizer of the following function:

$$\begin{aligned}
F(\Delta) &= -\hat{\Sigma}_{Y X_J} (w_J + \lambda_n \Delta) + \frac{1}{2} (w_J + \lambda_n \Delta)^\top \hat{\Sigma}_{X_J X_J} (w_J + \lambda_n \Delta) + \lambda_n \sum_{j \in J} d_j \|w_j + \lambda_n \Delta_j\| \\
&= -\lambda_n \hat{\Sigma}_{Y X_J} \Delta + \frac{\lambda_n^2}{2} \Delta^\top \hat{\Sigma}_{X_J X_J} \Delta + \lambda_n w_J^\top \hat{\Sigma}_{X_J X_J} \Delta + \lambda_n \sum_{j \in J} d_j (\|w_j + \lambda_n \Delta_j\| - \|w_j\|) + \text{cst} \\
&= -\lambda_n \hat{\Sigma}_{\varepsilon X_J} \Delta + \frac{\lambda_n^2}{2} \Delta^\top \hat{\Sigma}_{X_J X_J} \Delta + \lambda_n \sum_{j \in J} d_j (\|w_j + \lambda_n \Delta_j\| - \|w_j\|) + \text{cst},
\end{aligned}$$

by using $\hat{\Sigma}_{YX_J} = \mathbf{w}_J^\top \hat{\Sigma}_{X_J X_J} + \hat{\Sigma}_{\varepsilon X_J}$. The first term is $O_p(n^{-1/2} \lambda_n) = o_p(\lambda_n^2)$, while the last ones are equal to $\|\mathbf{w}_j + \lambda_n \Delta_j\| - \|\mathbf{w}_j\| = \lambda_n \left(\frac{\mathbf{w}_j}{\|\mathbf{w}_j\|} \right)^\top \Delta_j + o_p(\lambda_n)$. Thus,

$$F(\Delta)/\lambda_n^2 = \frac{1}{2} \Delta^\top \Sigma_{X_J X_J} \Delta + \sum_{j \in \mathbf{J}} \frac{d_j \mathbf{w}_j^\top}{\|\mathbf{w}_j\|} \Delta_j + o_p(1).$$

By Lemma 20, \hat{w}_J is $O_p(1)$ and the limiting function has an unique minimum; standard results in M-estimation (Van der Vaart, 1998) shows that $\hat{\Delta}$ converges in probability to the minimum of the last expression which is exactly $\Delta = -\Sigma_{X_J X_J}^{-1} \text{Diag}(d_j/\|\mathbf{w}_j\|) \mathbf{w}_J$. \blacksquare

We now turn to the proof of Theorem 4. We follow the proof of Theorem 2. Given \tilde{w} defined through Lemma 20 and 21, we need to satisfy optimality condition (2) for all $i \in \mathbf{J}^c$, with probability tending to one. For all those i such that $\frac{1}{d_i} \left\| \Sigma_{X_i X_J} \Sigma_{X_J X_J}^{-1} \text{Diag}(d_j/\|\mathbf{w}_j\|) \mathbf{w}_J \right\| < 1$, then we know from Appendix B.1, that the optimality condition is indeed satisfied with probability tending to one. We now focus on those i such that $\frac{1}{d_i} \left\| \Sigma_{X_i X_J} \Sigma_{X_J X_J}^{-1} \text{Diag}(d_j/\|\mathbf{w}_j\|) \mathbf{w}_J \right\| = 1$, and for which we have the condition in Eq. (6). From Eq. (35) and the few arguments that follow, we get that for all $i \in \mathbf{J}^c$,

$$\hat{\Sigma}_{X_i Y} - \hat{\Sigma}_{X_i X_J} \tilde{w}_J = \lambda_n \Sigma_{X_i X_J} \Sigma_{X_J X_J}^{-1} \text{Diag}(d_j/\|\tilde{w}_j\|) \tilde{w}_J + O_p(n^{-1/2}) \quad (36)$$

Moreover, we have from Lemma 21 and standard differential calculus, i.e., the gradient and the Hessian of the function $v \in \mathbb{R}^q \mapsto \|v\| \in \mathbb{R}$ are $v/\|v\|$ and $\frac{1}{\|v\|} \left(I_q - \frac{vv^\top}{v^\top v} \right)$:

$$\frac{\tilde{w}_j}{\|\tilde{w}_j\|} = \frac{\mathbf{w}_j}{\|\mathbf{w}_j\|} + \frac{\lambda_n}{\|\mathbf{w}_j\|} \left(I_{p_j} - \frac{\mathbf{w}_j \mathbf{w}_j^\top}{\mathbf{w}_j^\top \mathbf{w}_j} \right) \Delta_j + o_p(\lambda_n). \quad (37)$$

From Eq. (36) and Eq. (37), we get:

$$\begin{aligned} \frac{1}{\lambda_n} (\hat{\Sigma}_{X_i Y} - \hat{\Sigma}_{X_i X_J} \tilde{w}_J) &= O_p(n^{-1/2} \lambda_n^{-1}) + \Sigma_{X_i X_J} \Sigma_{X_J X_J}^{-1} \\ &\left\{ \text{Diag}(d_j/\|\mathbf{w}_j\|) \mathbf{w}_J + \lambda_n \Sigma_{X_i X_J} \Sigma_{X_J X_J}^{-1} \text{Diag} \left[d_j/\|\mathbf{w}_j\| \left(I_{p_j} - \frac{\mathbf{w}_j \mathbf{w}_j^\top}{\mathbf{w}_j^\top \mathbf{w}_j} \right) \right] \Delta + o_p(\lambda_n) \right\} \\ &= A + \lambda_n B + o_p(\lambda_n) + O_p(n^{-1/2} \lambda_n^{-1}). \end{aligned}$$

Since $\lambda_n \gg n^{-1/4}$, we have $O_p(n^{-1/2} \lambda_n^{-1}) = o_p(\lambda_n)$. Thus, since we assumed that $\|A\| = \|\Sigma_{X_i X_J} \Sigma_{X_J X_J}^{-1} \text{Diag}(d_j/\|\mathbf{w}_j\|) \mathbf{w}_J\| = d_i$, we have:

$$\begin{aligned} \left\| \frac{1}{\lambda_n} (\hat{\Sigma}_{X_i Y} - \hat{\Sigma}_{X_i X_J} \tilde{w}_J) \right\|^2 &= \|A\|^2 + 2\lambda_n A^\top B + o_p(\lambda_n) d_i^2 + o_p(\lambda_n) \\ &= d_i^2 + o_p(\lambda_n) \\ &\quad - 2\lambda_n \Delta^\top \Sigma_{X_J X_i} \Sigma_{X_i X_J} \Sigma_{X_J X_J}^{-1} \text{Diag} \left(d_j/\|\mathbf{w}_j\| \left(I_{p_j} - \frac{\mathbf{w}_j \mathbf{w}_j^\top}{\mathbf{w}_j^\top \mathbf{w}_j} \right) \right) \Delta, \end{aligned}$$

(note that we have $A = -\Sigma_{X_i X_J} \Delta$) which is asymptotically strictly smaller than d_i^2 if Eq. (6) is satisfied, which proves optimality and concludes the proof.

B.4 Proof of Proposition 6

As in the proof of Theorem 2 in Appendix B.1, we consider the estimate \tilde{w} built from the reduced problem by constraining $w_{\mathbf{J}^c} = 0$. We consider the following event:

$$E_1 = \{\hat{\Sigma}_{XX} \text{ invertible and } \forall j \in \mathbf{J}, \tilde{w}_j \neq 0\}.$$

This event has a probability converging to one. Moreover, if E_1 is true, then the group Lasso estimate has the correct sparsity pattern if and only if for all $i \in \mathbf{J}^c$,

$$\left\| \hat{\Sigma}_{X_i X_{\mathbf{J}}}(\tilde{w}_{\mathbf{J}} - \mathbf{w}_{\mathbf{J}}) - \hat{\Sigma}_{X_i \varepsilon} \right\| \leq \lambda_n d_i = \lambda_0 n^{-1/2} d_i.$$

Moreover we have by definition of $\tilde{w}_{\mathbf{J}}$: $\hat{\Sigma}_{X_{\mathbf{J}} X_{\mathbf{J}}}(\tilde{w}_{\mathbf{J}} - \mathbf{w}_{\mathbf{J}}) - \hat{\Sigma}_{X_{\mathbf{J}} \varepsilon} = -\lambda_n \text{Diag}(d_j / \|\tilde{w}_j\|) \tilde{w}_{\mathbf{J}}$, and thus, we get:

$$\begin{aligned} & \hat{\Sigma}_{X_i X_{\mathbf{J}}}(\tilde{w}_{\mathbf{J}} - \mathbf{w}_{\mathbf{J}}) - \hat{\Sigma}_{X_i \varepsilon} \\ &= \hat{\Sigma}_{X_i X_{\mathbf{J}}} \hat{\Sigma}_{X_{\mathbf{J}} X_{\mathbf{J}}}^{-1} \hat{\Sigma}_{X_{\mathbf{J}} \varepsilon} - \hat{\Sigma}_{X_i \varepsilon} - \lambda_0 n^{-1/2} \hat{\Sigma}_{X_i X_{\mathbf{J}}} \hat{\Sigma}_{X_{\mathbf{J}} X_{\mathbf{J}}}^{-1} \text{Diag}(d_j / \|\tilde{w}_j\|) \tilde{w}_{\mathbf{J}} \\ &= \Sigma_{X_i X_{\mathbf{J}}} \Sigma_{X_{\mathbf{J}} X_{\mathbf{J}}}^{-1} \hat{\Sigma}_{X_{\mathbf{J}} \varepsilon} - \hat{\Sigma}_{X_i \varepsilon} - \lambda_0 n^{-1/2} \Sigma_{X_i X_{\mathbf{J}}} \Sigma_{X_{\mathbf{J}} X_{\mathbf{J}}}^{-1} \text{Diag}(d_j / \|\mathbf{w}_j\|) \mathbf{w}_{\mathbf{J}} + O_p(n^{-1}) \end{aligned}$$

The random vector $\Sigma_{X_{\mathbf{J}} \varepsilon} \in \mathbb{R}^p$ is a multivariate U-statistic with square integrable kernel obtained from i.i.d. random vectors; it is thus asymptotically normal (Van der Vaart, 1998) and we simply need to compute its mean and variance. The mean is zero, and the variance is $\frac{n-1}{n^2} \sigma^2 \Sigma_{XX} = n^{-1} \sigma^2 \Sigma_{XX} + o(n^{-1})$. This implies that the random vector s of size $\text{Card}(\mathbf{J}^c)$ defined by

$$s_i = n^{1/2} \left\| \hat{\Sigma}_{X_i X_{\mathbf{J}}}(\tilde{w}_{\mathbf{J}} - \mathbf{w}_{\mathbf{J}}) - \hat{\Sigma}_{X_i \varepsilon} \right\|,$$

is equal to

$$\begin{aligned} s_i &= \left\| \sigma \Sigma_{X_i X_{\mathbf{J}}} \Sigma_{X_{\mathbf{J}} X_{\mathbf{J}}}^{-1} u_{\mathbf{J}} - \sigma u_i - \lambda_0 \Sigma_{X_i X_{\mathbf{J}}} \Sigma_{X_{\mathbf{J}} X_{\mathbf{J}}}^{-1} \text{Diag}(d_j / \|\mathbf{w}_j\|) \mathbf{w}_{\mathbf{J}} \right\| + O_p(n^{-1/2}) \\ &= f_i(u) + O_p(n^{-1/2}), \end{aligned}$$

where $u = \sigma^{-1} n^{-1/2} \hat{\Sigma}_{X_{\mathbf{J}} \varepsilon}$ and f_i are deterministic continuous functions. The vector $f(u)$ converges in distribution to $f(v)$ where v is normally distributed with mean zero and covariance matrix Σ_{XX} . By Slutsky's lemma (Van der Vaart, 1998), this implies that the random vector s has the same limiting distribution. Thus, the probability $\mathbb{P}(\max_{i \in \mathbf{J}^c} s_i / d_i \leq \lambda_0)$ converges to

$$\mathbb{P} \left(\max_{i \in \mathbf{J}^c} \frac{1}{d_i} \left\| \sigma (\Sigma_{X_i X_{\mathbf{J}}} \Sigma_{X_{\mathbf{J}} X_{\mathbf{J}}}^{-1} v_{\mathbf{J}} - v_i) - \lambda_0 \Sigma_{X_i X_{\mathbf{J}}} \Sigma_{X_{\mathbf{J}} X_{\mathbf{J}}}^{-1} \text{Diag}(d_j / \|\mathbf{w}_j\|) \mathbf{w}_{\mathbf{J}} \right\| \leq \lambda_0 \right).$$

Under the event E_1 which has probability tending to one, we have correct pattern selection if and only if $\max_{i \in \mathbf{J}^c} s_i / d_i \leq \lambda_0$, which leads to

$$\mathbb{P} \left(\max_{i \in \mathbf{J}^c} \frac{1}{d_i} \left\| \sigma t_i - \lambda_0 \Sigma_{X_i X_{\mathbf{J}}} \Sigma_{X_{\mathbf{J}} X_{\mathbf{J}}}^{-1} \text{Diag}(d_j / \|\mathbf{w}_j\|) \mathbf{w}_{\mathbf{J}} \right\| \leq \lambda_0 \right),$$

where $t_i = \Sigma_{X_i X_{\mathbf{J}}} \Sigma_{X_{\mathbf{J}} X_{\mathbf{J}}}^{-1} v_{\mathbf{J}} - v_i$. The vector t is normally distributed and a short calculation shows that its covariance matrix is equal to $\Sigma_{X_{\mathbf{J}^c} X_{\mathbf{J}^c} | X_{\mathbf{J}}}$, which concludes the proof.

Appendix C. Detailed Proofs for the Nonparametric Formulation

We first prove lemmas that will be useful for further proofs, and then prove the consistency results for the non parametric case.

C.1 Useful Lemmas on Empirical Covariance Operators

We first have the following lemma, proved by Fukumizu et al. (2007), which states that the empirical covariance estimator converges in probability at rate $O_p(n^{-1/2})$ to the population covariance operators:

Lemma 22 *Assume (A4) and (A6). Then $\|\hat{\Sigma}_{XX} - \Sigma_{XX}\|_{\mathcal{F}} = O_p(n^{-1/2})$ (for the operator norm), $\|\hat{\Sigma}_{XY} - \Sigma_{XY}\|_{\mathcal{F}} = O_p(n^{-1/2})$ and $\|\hat{\Sigma}_{X\varepsilon}\|_{\mathcal{F}} = O_p(n^{-1/2})$.*

The following lemma is useful in several proofs:

Lemma 23 *Assume (A4). Then $\left\| \left(\hat{\Sigma}_{XX} + \mu_n I \right)^{-1} \Sigma_{XX} - \left(\Sigma_{XX} + \mu_n I \right)^{-1} \Sigma_{XX} \right\|_{\mathcal{F}} = O_p(n^{-1/2} \mu_n^{-1})$, and $\left\| \left(\hat{\Sigma}_{XX} + \mu_n I \right)^{-1} \hat{\Sigma}_{XX} - \left(\Sigma_{XX} + \mu_n I \right)^{-1} \Sigma_{XX} \right\|_{\mathcal{F}} = O_p(n^{-1/2} \mu_n^{-1})$.*

Proof We have:

$$\begin{aligned} & \left(\hat{\Sigma}_{XX} + \mu_n I \right)^{-1} \Sigma_{XX} - \left(\Sigma_{XX} + \mu_n I \right)^{-1} \Sigma_{XX} \\ &= \left(\hat{\Sigma}_{XX} + \mu_n I \right)^{-1} \left(\Sigma_{XX} - \hat{\Sigma}_{XX} \right) \left(\Sigma_{XX} + \mu_n I \right)^{-1} \Sigma_{XX} \end{aligned}$$

This is the product of operators whose norms are respectively upper bounded by μ_n^{-1} , $O_p(n^{-1/2})$ and 1, which leads to the first inequality (we use $\|AB\|_{\mathcal{F}} \leq \|A\|_{\mathcal{F}} \|B\|_{\mathcal{F}}$). The second inequality follows along similar lines. \blacksquare

Note that the two previous lemma also hold for any suboperator of Σ_{XX} , i.e., for $\Sigma_{X_j X_j}$, or $\Sigma_{X_i X_i}$.

Lemma 24 *Assume (A4), (A5) and (A7). There exists $\mathbf{h}_J \in \mathcal{F}_J$ such that $\mathbf{f}_J = \Sigma_{X_j X_j}^{1/2} \mathbf{h}_J$.*

Proof The range condition implies that

$$\mathbf{f}_J = \text{Diag}(\Sigma_{X_j X_j}^{1/2}) \mathbf{g}_J = \text{Diag}(\Sigma_{X_j X_j}^{1/2}) C_{X_j X_j}^{1/2} C_{X_j X_j}^{-1/2} \mathbf{g}_J$$

(because $C_{X_j X_j}$ is invertible). The result follows from the identity

$$\Sigma_{X_j X_j} = \text{Diag}(\Sigma_{X_j X_j}^{1/2}) C_{X_j X_j}^{1/2} \left(\text{Diag}(\Sigma_{X_j X_j}^{1/2}) C_{X_j X_j}^{1/2} \right)^*$$

and the fact that if $\Sigma_{X_j X_j} = UU^*$ and $f = U\alpha$ then there exists β such that $f = \Sigma_{X_j X_j}^{1/2} \beta$ (Baker, 1973).⁴ \blacksquare

4. The adjoint operator V^* of $V : \mathcal{F}_i \rightarrow \mathcal{F}_j$ is so that for all $f \in \mathcal{F}_i$ and $g \in \mathcal{F}_j$, $\langle f, Vg \rangle_{\mathcal{F}_i} = \langle V^*f, g \rangle_{\mathcal{F}_j}$ (Brezis, 1980).

C.2 Proof of Theorem 11

We now extend Lemma 20 to covariance operators, which requires to use the alternative formulation and a slower rate of decrease for the regularization parameter:

Lemma 25 *Let $\tilde{f}_{\mathbf{J}}$ be any minimizer of*

$$\frac{1}{2}\hat{\Sigma}_{YY} - \langle \hat{\Sigma}_{XJY}, f_{\mathbf{J}} \rangle_{\mathcal{F}_{\mathbf{J}}} + \frac{1}{2}\langle f_{\mathbf{J}}, \hat{\Sigma}_{XJXJ} f_{\mathbf{J}} \rangle_{\mathcal{F}_{\mathbf{J}}} + \frac{\mu_n}{2} \left(\sum_{j \in \mathbf{J}} d_j \|f_j\|_{\mathcal{F}_j} \right)^2.$$

If $\mu_n \rightarrow 0$ and $\mu_n n^{1/2} \rightarrow +\infty$, then $\|\tilde{f}_{\mathbf{J}} - \mathbf{f}_{\mathbf{J}}\|_{\mathcal{F}_{\mathbf{J}}}$ converges to zero in probability. Moreover for any η_n such that $\eta_n \gg \mu_n^{1/2} + \mu_n^{-1} n^{-1/2}$ then $\|\tilde{f}_{\mathbf{J}} - \mathbf{f}_{\mathbf{J}}\|_{\mathcal{F}_{\mathbf{J}}} = O_p(\eta_n)$.

Proof Note that from Cauchy-Schwartz inequality, we have:

$$\begin{aligned} \left(\sum_{j \in \mathbf{J}} d_j \|f_j\|_{\mathcal{F}_j} \right)^2 &= \left(\sum_{j \in \mathbf{J}} d_j^{1/2} \|\mathbf{f}_j\|_{\mathcal{F}_j}^{1/2} \times \frac{d_j^{1/2} \|f_j\|_{\mathcal{F}_j}}{\|\mathbf{f}_j\|_{\mathcal{F}_j}^{1/2}} \right)^2 \\ &\leq \left(\sum_{j \in \mathbf{J}} d_j \|\mathbf{f}_j\|_{\mathcal{F}_j} \right) \sum_{j \in \mathbf{J}} \frac{d_j \|f_j\|_{\mathcal{F}_j}^2}{\|\mathbf{f}_j\|_{\mathcal{F}_j}}, \end{aligned}$$

with equality if and only if there exists $\alpha > 0$ such that $\|f_j\|_{\mathcal{F}_j} = \alpha \|\mathbf{f}_j\|_{\mathcal{F}_j}$ for all $j \in \mathbf{J}$. We consider the unique minimizer $\bar{f}_{\mathbf{J}}$ of the following cost function, built by replacing the regularization by its upperbound,

$$F(f_{\mathbf{J}}) = \frac{1}{2}\hat{\Sigma}_{YY} - \langle \hat{\Sigma}_{XJY}, f_{\mathbf{J}} \rangle_{\mathcal{F}_{\mathbf{J}}} + \frac{1}{2}\langle f_{\mathbf{J}}, \hat{\Sigma}_{XJXJ} f_{\mathbf{J}} \rangle_{\mathcal{F}_{\mathbf{J}}} + \frac{\mu_n}{2} \left(\sum_{j \in \mathbf{J}} d_j \|\mathbf{f}_j\|_{\mathcal{F}_j} \right) \sum_{j \in \mathbf{J}} \frac{d_j \|f_j\|_{\mathcal{F}_j}^2}{\|\mathbf{f}_j\|_{\mathcal{F}_j}}.$$

Since it is a regularized least-square problem, we have (with $\varepsilon = Y - \sum_{j \in \mathbf{J}} \mathbf{f}_j(X) - \mathbf{b}$):

$$\bar{f}_{\mathbf{J}} = \left(\hat{\Sigma}_{XJXJ} + \mu_n D \right)^{-1} \left(\hat{\Sigma}_{XJXJ} \mathbf{f}_{\mathbf{J}} + \hat{\Sigma}_{XJ\varepsilon} \right),$$

where $D = \left(\sum_{j \in \mathbf{J}} d_j \|\mathbf{f}_j\| \right) \text{Diag}(d_j / \|\mathbf{f}_j\|)$. Note that D is upperbounded and lowerbounded, as an auto-adjoint operator, by *strictly positive* constants times the identity operator (with probability tending to one), i.e., $D_{\max} I_{\mathcal{F}_{\mathbf{J}}} \succcurlyeq D \succcurlyeq D_{\min} I_{\mathcal{F}_{\mathbf{J}}}$ with $D_{\min}, D_{\max} > 0$. We now prove that $\bar{f}_{\mathbf{J}} - \mathbf{f}_{\mathbf{J}}$ is converging to zero in probability. We have:

$$\left(\hat{\Sigma}_{XJXJ} + \mu_n D \right)^{-1} \hat{\Sigma}_{XJ\varepsilon} = O_p(n^{-1/2} \mu_n^{-1}), \quad (38)$$

because of Lemma 22 and $\left\| \left(\hat{\Sigma}_{XJXJ} + \mu_n D \right)^{-1} \right\|_{\mathcal{F}_{\mathbf{J}}} \leq D_{\min}^{-1} \mu_n^{-1}$. Moreover, similarly, we have

$$\left(\hat{\Sigma}_{XJXJ} + \mu_n D \right)^{-1} \hat{\Sigma}_{XJXJ} f_{\mathbf{J}} - \left(\hat{\Sigma}_{XJXJ} + \mu_n D \right)^{-1} \hat{\Sigma}_{XJXJ} \mathbf{f}_{\mathbf{J}} = O_p(n^{-1/2} \mu_n^{-1}). \quad (39)$$

Besides, by Lemma 23,

$$\left(\hat{\Sigma}_{X_{\mathbf{J}}X_{\mathbf{J}}} + \mu_n D\right)^{-1} \Sigma_{X_{\mathbf{J}}X_{\mathbf{J}}} f_{\mathbf{J}} - (\Sigma_{X_{\mathbf{J}}X_{\mathbf{J}}} + \mu_n D)^{-1} \Sigma_{X_{\mathbf{J}}X_{\mathbf{J}}} f_{\mathbf{J}} = O_p(n^{-1/2} \mu_n^{-1}). \quad (40)$$

Thus $\bar{f}_{\mathbf{J}} - \mathbf{f}_{\mathbf{J}} = V + O_p(n^{-1/2} \mu_n^{-1})$, where

$$V = \left[(\Sigma_{X_{\mathbf{J}}X_{\mathbf{J}}} + \mu_n D)^{-1} \Sigma_{X_{\mathbf{J}}X_{\mathbf{J}}} - I \right] \mathbf{f}_{\mathbf{J}} = -(\Sigma_{X_{\mathbf{J}}X_{\mathbf{J}}} + \mu_n D)^{-1} \mu_n D \mathbf{f}_{\mathbf{J}}.$$

We have

$$\begin{aligned} \|V\|_{\mathcal{F}_{\mathbf{J}}}^2 &= \mu_n^2 \langle \mathbf{f}_{\mathbf{J}}, D (\Sigma_{X_{\mathbf{J}}X_{\mathbf{J}}} + \mu_n D)^{-2} D \mathbf{f}_{\mathbf{J}} \rangle_{\mathcal{F}_{\mathbf{J}}} \\ &\leq D_{\max}^2 \mu_n^2 \langle \mathbf{f}_{\mathbf{J}}, (\Sigma_{X_{\mathbf{J}}X_{\mathbf{J}}} + \mu_n D_{\min} I)^{-2} \mathbf{f}_{\mathbf{J}} \rangle_{\mathcal{F}_{\mathbf{J}}} \\ &\leq D_{\max}^2 \mu_n \langle \mathbf{f}_{\mathbf{J}}, (\Sigma_{X_{\mathbf{J}}X_{\mathbf{J}}} + \mu_n D_{\min} I)^{-1} \mathbf{f}_{\mathbf{J}} \rangle_{\mathcal{F}_{\mathbf{J}}} \\ &\leq D_{\max}^2 \mu_n \langle \mathbf{h}_{\mathbf{J}}, \Sigma_{X_{\mathbf{J}}X_{\mathbf{J}}} (\Sigma_{X_{\mathbf{J}}X_{\mathbf{J}}} + \mu_n D_{\min} I)^{-1} \mathbf{h}_{\mathbf{J}} \rangle_{\mathcal{F}_{\mathbf{J}}} \text{ by Lemma 24,} \\ &\leq D_{\max}^2 \mu_n \|\mathbf{h}_{\mathbf{J}}\|_{\mathcal{F}_{\mathbf{J}}}^2. \end{aligned}$$

Finally we obtain $\|\bar{f}_{\mathbf{J}} - \mathbf{f}_{\mathbf{J}}\|_{\mathcal{F}_{\mathbf{J}}} = O_p(\mu_n^{1/2} + n^{-1/2} \mu_n^{-1})$.

We now consider the cost function defining $\tilde{f}_{\mathbf{J}}$:

$$F_n(f_{\mathbf{J}}) = \frac{1}{2} \hat{\Sigma}_{Y Y} - \langle \hat{\Sigma}_{X_{\mathbf{J}} Y}, f_{\mathbf{J}} \rangle_{\mathcal{F}_{\mathbf{J}}} + \frac{1}{2} \langle f_{\mathbf{J}}, \hat{\Sigma}_{X_{\mathbf{J}} X_{\mathbf{J}}} f_{\mathbf{J}} \rangle_{\mathcal{F}_{\mathbf{J}}} + \frac{\mu_n}{2} \left(\sum_{j \in \mathbf{J}} d_j \|f_j\|_{\mathcal{F}_j} \right)^2.$$

We have (note that although we seem to take infinite dimensional derivatives, everything can be done in the finite subspace spanned by the data):

$$\begin{aligned} F_n(f_{\mathbf{J}}) - F(f_{\mathbf{J}}) &= \frac{\mu_n}{2} \left[\left(\sum_{j \in \mathbf{J}} d_j \|f_j\|_{\mathcal{F}_j} \right)^2 - \left(\sum_{j \in \mathbf{J}} d_j \|\mathbf{f}_j\|_{\mathcal{F}_j} \right) \sum_{j \in \mathbf{J}} \frac{d_j \|f_j\|_{\mathcal{F}_j}^2}{\|\mathbf{f}_j\|_{\mathcal{F}_j}} \right], \\ \nabla_{f_i} F_n(f_{\mathbf{J}}) - \nabla_{f_i} F(f_{\mathbf{J}}) &= \mu_n \left[\left(\sum_{j \in \mathbf{J}} d_j \|f_j\|_{\mathcal{F}_j} \right) \frac{d_i f_i}{\|f_i\|_{\mathcal{F}_j}} - \left(\sum_{j \in \mathbf{J}} d_j \|\mathbf{f}_j\|_{\mathcal{F}_j} \right) \frac{d_i f_i}{\|\mathbf{f}_i\|_{\mathcal{F}_j}} \right]. \end{aligned}$$

Since the right hand side of the previous equation corresponds to a continuously differentiable function of $f_{\mathbf{J}}$ around $\mathbf{f}_{\mathbf{J}}$ (with upper-bounded derivatives around $\mathbf{f}_{\mathbf{J}}$), we have:

$$\|\nabla_{f_i} F_n(\bar{f}_{\mathbf{J}}) - 0\|_{\mathcal{F}_i} \leq C \mu_n \|\mathbf{f}_{\mathbf{J}} - \bar{f}_{\mathbf{J}}\|_{\mathcal{F}_{\mathbf{J}}} = \mu_n O_p(\mu_n^{1/2} + n^{-1/2} \mu_n^{-1}).$$

for some constant $C > 0$. Moreover, on the ball of center $\bar{f}_{\mathbf{J}}$ and radius η_n such that $\eta_n \gg \mu_n^{1/2} + \mu_n^{-1} n^{-1/2}$ (to make sure that it asymptotically contains $\mathbf{f}_{\mathbf{J}}$, which implies that on the ball each $f_j, j \in \mathbf{J}$ are bounded away from zero), and $\eta_n \ll 1$ (so that we get consistency), we have a lower bound on the second derivative of $\left(\sum_{j \in \mathbf{J}} d_j \|f_j\|_{\mathcal{F}_j} \right)$. Thus for any element of the ball,

$$F_n(f_{\mathbf{J}}) \geq F_n(\bar{f}_{\mathbf{J}}) + \langle \nabla_{f_{\mathbf{J}}} F_n(\bar{f}_{\mathbf{J}}), (f_{\mathbf{J}} - \bar{f}_{\mathbf{J}}) \rangle_{\mathcal{F}_{\mathbf{J}}} + C' \mu_n \|f_{\mathbf{J}} - \bar{f}_{\mathbf{J}}\|_{\mathcal{F}_{\mathbf{J}}}^2,$$

where $C' > 0$ is a constant. This implies that the value of $F_n(f_{\mathbf{J}})$ on the edge of the ball is larger than

$$F_n(\bar{f}_{\mathbf{J}}) + \eta_n \mu_n O_p(\mu_n^{1/2} + n^{-1/2} \mu_n^{-1}) + C' \eta_n^2 \mu_n,$$

Thus if $\eta_n^2 \mu_n \gg \eta_n \mu_n^{3/2}$ and $\eta_n^2 \mu_n \gg n^{-1/2} \eta_n$, then we must have all minima inside the ball of radius η_n (because with probability tending to one, the value on the edge is greater than one value inside and the function is convex) which implies that the global minimum of F_n is at most η_n away from $\bar{f}_{\mathbf{J}}$ and thus since $\bar{f}_{\mathbf{J}}$ is $O(\mu_n^{1/2})$ away from $\mathbf{f}_{\mathbf{J}}$, we have the consistency if

$$\eta_n \ll 1 \text{ and } \eta_n \gg \mu_n^{1/2} + n^{-1/2} \mu_n^{-1},$$

which concludes the proof of the lemma. ■

We now prove Theorem 11. Let $\tilde{f}_{\mathbf{J}}$ be defined as in Lemma 20. We extend it by zeros on \mathbf{J}^c . We already know the squared norm consistency by Lemma 20. Since by Proposition 14, the solution is unique with probability tending to one, we need to prove that with probability tending to one \tilde{f} is optimal for problem in Eq. (15). We have by the first optimality condition for $\tilde{f}_{\mathbf{J}}$:

$$\hat{\Sigma}_{X_{\mathbf{J}}Y} - \hat{\Sigma}_{X_{\mathbf{J}}X_{\mathbf{J}}} \tilde{f}_{\mathbf{J}} = \mu_n \| \tilde{f} \|_d \text{Diag}(d_j / \| \tilde{f}_j \|) \tilde{f}_{\mathbf{J}},$$

where we use the notation $\|f\|_d = \sum_{j=1}^m d_j \|f_j\|_{\mathcal{F}_j}$ (note the difference with $\|f\|_{\mathcal{F}} = (\sum_{j=1}^m \|f_j\|_{\mathcal{F}_j}^2)^{1/2}$). We thus have by solving for $\tilde{f}_{\mathbf{J}}$ and using $\hat{\Sigma}_{X_{\mathbf{J}}Y} = \hat{\Sigma}_{X_{\mathbf{J}}X_{\mathbf{J}}} \mathbf{f}_{\mathbf{J}} + \hat{\Sigma}_{X_{\mathbf{J}}\varepsilon}$:

$$\tilde{f}_{\mathbf{J}} = \left(\hat{\Sigma}_{X_{\mathbf{J}}X_{\mathbf{J}}} + \mu_n D_n \right)^{-1} \left(\hat{\Sigma}_{X_{\mathbf{J}}X_{\mathbf{J}}} \mathbf{f}_{\mathbf{J}} + \hat{\Sigma}_{X_{\mathbf{J}}\varepsilon} \right),$$

with the notation $D_n = \| \tilde{f} \|_d \text{Diag}(d_j / \| \tilde{f}_j \|_{\mathcal{F}_j})$. We can now put that back into $\hat{\Sigma}_{X_{\mathbf{J}}^c Y} - \hat{\Sigma}_{X_{\mathbf{J}}^c X_{\mathbf{J}}} \tilde{f}_{\mathbf{J}}$ and show that this will have small enough norm with probability tending to one. We have for all $i \in \mathbf{J}^c$:

$$\begin{aligned} \hat{\Sigma}_{X_i Y} - \hat{\Sigma}_{X_i X_{\mathbf{J}}} \tilde{f}_{\mathbf{J}} &= \hat{\Sigma}_{X_i Y} - \hat{\Sigma}_{X_i X_{\mathbf{J}}} \left(\hat{\Sigma}_{X_{\mathbf{J}}X_{\mathbf{J}}} + \mu_n D_n \right)^{-1} \left(\hat{\Sigma}_{X_{\mathbf{J}}X_{\mathbf{J}}} \mathbf{f}_{\mathbf{J}} + \hat{\Sigma}_{X_{\mathbf{J}}\varepsilon} \right) \\ &= -\hat{\Sigma}_{X_i X_{\mathbf{J}}} \left(\hat{\Sigma}_{X_{\mathbf{J}}X_{\mathbf{J}}} + \mu_n D_n \right)^{-1} \hat{\Sigma}_{X_{\mathbf{J}}X_{\mathbf{J}}} \mathbf{f}_{\mathbf{J}} \\ &\quad + \hat{\Sigma}_{X_i Y} - \hat{\Sigma}_{X_i X_{\mathbf{J}}} \left(\hat{\Sigma}_{X_{\mathbf{J}}X_{\mathbf{J}}} + \mu_n D_n \right)^{-1} \hat{\Sigma}_{X_{\mathbf{J}}\varepsilon} \\ &= -\hat{\Sigma}_{X_i X_{\mathbf{J}}} \mathbf{f}_{\mathbf{J}} + \hat{\Sigma}_{X_i X_{\mathbf{J}}} \left(\hat{\Sigma}_{X_{\mathbf{J}}X_{\mathbf{J}}} + \mu_n D_n \right)^{-1} \mu_n D_n \mathbf{f}_{\mathbf{J}} \\ &\quad + \hat{\Sigma}_{X_i Y} - \hat{\Sigma}_{X_i X_{\mathbf{J}}} \left(\hat{\Sigma}_{X_{\mathbf{J}}X_{\mathbf{J}}} + \mu_n D_n \right)^{-1} \hat{\Sigma}_{X_{\mathbf{J}}\varepsilon} \\ &= \hat{\Sigma}_{X_i X_{\mathbf{J}}} \left(\hat{\Sigma}_{X_{\mathbf{J}}X_{\mathbf{J}}} + \mu_n D_n \right)^{-1} \mu_n D_n \mathbf{f}_{\mathbf{J}} \\ &\quad + \hat{\Sigma}_{X_i \varepsilon} - \hat{\Sigma}_{X_i X_{\mathbf{J}}} \left(\hat{\Sigma}_{X_{\mathbf{J}}X_{\mathbf{J}}} + \mu_n D_n \right)^{-1} \hat{\Sigma}_{X_{\mathbf{J}}\varepsilon} \\ &= A_n + B_n. \end{aligned} \tag{41}$$

The first term A_n (divided by μ_n) is equal to

$$\frac{A_n}{\mu_n} = \hat{\Sigma}_{X_i X_{\mathbf{J}}} \left(\hat{\Sigma}_{X_{\mathbf{J}}X_{\mathbf{J}}} + \mu_n D_n \right)^{-1} D_n \mathbf{f}_{\mathbf{J}}.$$

We can replace $\hat{\Sigma}_{X_i X_J}$ in $\frac{A_n}{\mu_n}$ by $\Sigma_{X_i X_J}$ at cost $O_p(n^{-1/2} \mu_n^{-1/2})$ because $\langle \mathbf{f}_J, \Sigma_{X_J X_J}^{-1} \mathbf{f}_J \rangle_{\mathcal{F}_J} < \infty$ (by Lemma 24). Also, we can replace $\hat{\Sigma}_{X_J X_J}$ in $\frac{A_n}{\mu_n}$ by $\Sigma_{X_J X_J}$ at cost $O_p(n^{-1/2} \mu_n^{-1})$ as a consequence of Lemma 23. Those two are $o_p(1)$ by assumptions on μ_n . Thus,

$$\frac{A_n}{\mu_n} = \Sigma_{X_i X_J} (\Sigma_{X_J X_J} + \mu_n D_n)^{-1} D_n \mathbf{f}_J + o_p(1).$$

Furthermore, we let denote $D = \|\mathbf{f}\|_d \text{Diag}(d_j / \|\mathbf{f}_j\|_{\mathcal{F}_j})$. From Lemma 25, we know that $D_n - D = o_p(1)$. Thus we can replace D_n by D at cost $o_p(1)$ to get:

$$\frac{A_n}{\mu_n} = \Sigma_{X_i X_J} (\Sigma_{X_J X_J} + \mu_n D)^{-1} D \mathbf{f}_J + o_p(1) = C_n + o_p(1).$$

We now show that this last deterministic term $C_n \in \mathcal{F}_i$ converges to:

$$C = \Sigma_{X_i X_i}^{1/2} C_{X_i X_J} C_{X_J X_J}^{-1} D \mathbf{g}_J,$$

where, from (A7), $\forall j \in \mathbf{J}$, $\mathbf{f}_j = \Sigma_{X_j X_j}^{1/2} \mathbf{g}_j$. We have

$$\begin{aligned} C_n - C &= \Sigma_{X_i X_i}^{1/2} C_{X_i X_J} \left[\text{Diag}(\Sigma_{X_j X_j}^{1/2}) (\Sigma_{X_J X_J} + \mu_n D)^{-1} \text{Diag}(\Sigma_{X_j X_j}^{1/2}) - C_{X_J X_J}^{-1} \right] D \mathbf{g}_J \\ &= \Sigma_{X_i X_i}^{1/2} C_{X_i X_J} K_n D \mathbf{g}_J. \end{aligned}$$

where $K_n = \text{Diag}(\Sigma_{X_j X_j}^{1/2}) (\Sigma_{X_J X_J} + \mu_n D)^{-1} \text{Diag}(\Sigma_{X_j X_j}^{1/2}) - C_{X_J X_J}^{-1}$. In addition, we have:

$$\begin{aligned} \text{Diag}(\Sigma_{X_j X_j}^{1/2}) C_{X_J X_J} K_n &= \Sigma_{X_J X_J} (\Sigma_{X_J X_J} + \mu_n D)^{-1} \text{Diag}(\Sigma_{X_j X_j}^{1/2}) - \text{Diag}(\Sigma_{X_j X_j}^{1/2}) \\ &= -\mu_n D (\Sigma_{X_J X_J} + \mu_n D)^{-1} \text{Diag}(\Sigma_{X_j X_j}^{1/2}). \end{aligned}$$

Following Fukumizu et al. (2007), the range of the adjoint operator $\left(\Sigma_{X_i X_i}^{1/2} C_{X_i X_J} \right)^* = C_{X_J X_i} \Sigma_{X_i X_i}^{1/2}$ is included in the closure of the range of $\text{Diag}(\Sigma_{X_j X_j})$ (which is equal to the range of $\Sigma_{X_J X_J}$ by Lemma 24). For any $v_J \in \mathcal{F}_J$ in the intersection of two ranges, we have $v_J = C_{X_J X_J} \text{Diag}(\Sigma_{X_j X_j}^{1/2}) u_J$ (note that $C_{X_J X_J}$ is invertible), and thus

$$\begin{aligned} \langle K_n D \mathbf{g}_J, v_J \rangle_{\mathcal{F}_J} &= \langle K_n D \mathbf{g}_J, C_{X_J X_J} \text{Diag}(\Sigma_{X_j X_j}^{1/2}) u_J \rangle_{\mathcal{F}_J} \\ &= \langle -\mu_n D (\Sigma_{X_J X_J} + \mu_n D)^{-1} \text{Diag}(\Sigma_{X_j X_j}^{1/2}) D \mathbf{g}_J, u_J \rangle_{\mathcal{F}_J} \end{aligned}$$

which is $O_p(\mu_n^{1/2})$ and thus tends to zero. Since this holds for all elements in the intersection of the ranges, Lemma 9 by Fukumizu et al. (2007) implies that $\|C_n - C\|_{\mathcal{F}_J}$ converges to zero.

We now simply need to show that the second term B_n is dominated by μ_n . We have: $\|\hat{\Sigma}_{X_i \varepsilon}\|_{\mathcal{F}_i} = O_p(n^{-1/2})$ and $\|\hat{\Sigma}_{X_i X_J} \left(\hat{\Sigma}_{X_J X_J} + \mu_n D_n \right)^{-1} \hat{\Sigma}_{X_J \varepsilon}\|_{\mathcal{F}_i} \leq \|\hat{\Sigma}_{X_i \varepsilon}\|_{\mathcal{F}_i}$, thus, since $\mu_n n^{1/2} \rightarrow +\infty$, $B_n = o_p(\mu_n)$ and therefore for for each $i \in J^c$,

$$\frac{1}{d_i \mu_n \|\mathbf{f}\|_d} \left(\hat{\Sigma}_{X_i Y} - \hat{\Sigma}_{X_i X_J} \tilde{f}_J \right)$$

converges in probability to $\|C\|_{\mathcal{F}_J}/d_i\|\mathbf{f}\|_d$ which is strictly smaller than one because Eq. (18) is satisfied. Thus

$$\mathbb{P}\left\{\frac{1}{d_i\mu_n\|\mathbf{f}\|_d}\left\|\hat{\Sigma}_{X_iY} - \hat{\Sigma}_{X_iX_J}\hat{f}_J\right\|_{\mathcal{F}_i} \leq 1\right\}$$

is tending to 1, which implies the theorem (using the same arguments than in the proof of Theorem 2 in Appendix B.1).

C.3 Proof of Theorem 12

Before proving the analog of the second group Lasso theorem, we need the following additional proposition, which states that consistency of the patterns can only be achieved if $\mu_n n^{1/2} \rightarrow \infty$ (even if chosen in a data dependent way).

Proposition 26 *Assume (A4-7) and that \mathbf{J} is not empty. If \hat{f} is converging in probability to \mathbf{f} and $J(\hat{f})$ converges in probability to \mathbf{J} , then $\mu_n n^{1/2} \rightarrow \infty$ in probability.*

Proof We give a proof by contradiction, and we thus assume that there exists $M > 0$ such that $\liminf_{n \rightarrow \infty} \mathbb{P}(\mu_n n^{1/2} < M) > 0$. This imposes that there exists a subsequence which is almost surely bounded by M (Durrett, 2004). Thus, we can take a further subsequence which converges to a limit $\mu_0 \in [0, \infty)$. We now consider such a subsequence (and still use the notation of the original sequence for simplicity).

With probability tending to one, we have the optimality condition (17):

$$\hat{\Sigma}_{X_J\epsilon} + \hat{\Sigma}_{X_JX_J}\mathbf{f}_J = \hat{\Sigma}_{X_JY} = \hat{\Sigma}_{X_JX_J}\hat{f}_J + \mu_n\|\hat{f}\|_d \text{Diag}(d_j/\|\hat{f}_j\|_{\mathcal{F}_j})\hat{f}_J.$$

If we let denote $D_n = n^{1/2}\mu_n\|\hat{f}\|_d \text{Diag}(d_j/\|\hat{f}_j\|_{\mathcal{F}_j})$, we get:

$$D_n\mathbf{f}_J = \left[\hat{\Sigma}_{X_JX_J} + D_n n^{-1/2}\right] n^{1/2} \left[\mathbf{f}_J - \hat{f}_J\right] + n^{1/2}\hat{\Sigma}_{X_J\epsilon},$$

which can be approximated as follows (we denote $D = \|\mathbf{f}\|_d \text{Diag}(d_j/\|\mathbf{f}_j\|_{\mathcal{F}_j})$):

$$\mu_0 D\mathbf{f}_J + o_p(1) = \Sigma_{X_JX_J} n^{1/2} \left[\mathbf{f}_J - \hat{f}_J\right] + o_p(1) + n^{1/2}\hat{\Sigma}_{X_J\epsilon}.$$

We can now write for $i \in \mathbf{J}^c$:

$$\begin{aligned} n^{1/2} \left(\hat{\Sigma}_{X_iY} - \hat{\Sigma}_{X_iX_J}\hat{f}_J\right) &= n^{1/2}\hat{\Sigma}_{X_i\epsilon} + \hat{\Sigma}_{X_iX_J} n^{1/2}(\mathbf{f}_J - \hat{f}_J) \\ &= n^{1/2}\hat{\Sigma}_{X_i\epsilon} + \Sigma_{X_iX_J} n^{1/2}(\mathbf{f}_J - \hat{f}_J) + o_p(1). \end{aligned}$$

We now consider an arbitrary vector $w_J \in \mathcal{F}_J$, such that $\Sigma_{X_JX_J}w_J$ is different from zero (such vector exists because $\Sigma_{X_JX_J} \neq 0$, as we have assumed in (A4) that the variables are not constant). Since the range of $\Sigma_{X_JX_i}$ is included in the range of $\Sigma_{X_JX_J}$ (Baker, 1973), there exists $v_i \in \mathcal{F}_i$ such that $\Sigma_{X_JX_i}v_i = \Sigma_{X_JX_J}w_J$. Note that since $\Sigma_{X_JX_J}w_J$ is different from zero, we must have $\Sigma_{X_iX_i}^{1/2}v_i \neq 0$. We have:

$$\begin{aligned} n^{1/2}\langle v_i, \hat{\Sigma}_{X_iY} - \hat{\Sigma}_{X_iX_J}\hat{f}_J \rangle_{\mathcal{F}_i} &= n^{1/2}\langle v_i, \hat{\Sigma}_{X_i\epsilon} \rangle_{\mathcal{F}_i} + \langle w_J, \Sigma_{X_JX_J} n^{1/2}(\mathbf{f}_J - \hat{f}_J) \rangle_{\mathcal{F}_J} + o_p(1) \\ &= n^{1/2}\langle v_i, \hat{\Sigma}_{X_i\epsilon} \rangle_{\mathcal{F}_i} + \langle w_J, \mu_0 D\mathbf{f}_J - n^{1/2}\hat{\Sigma}_{X_J\epsilon} \rangle_{\mathcal{F}_J} + o_p(1) \\ &= \langle w_J, \mu_0 D\mathbf{f}_J \rangle_{\mathcal{F}_J} + n^{1/2}\langle v_i, \hat{\Sigma}_{X_i\epsilon} \rangle_{\mathcal{F}_i} - n^{1/2}\langle w_J, \hat{\Sigma}_{X_J\epsilon} \rangle_{\mathcal{F}_J} + o_p(1). \end{aligned}$$

The random variable $E_n = n^{1/2}\langle v_i, \hat{\Sigma}_{X_i\varepsilon} \rangle - n^{1/2}\langle w_{\mathbf{J}}, \hat{\Sigma}_{X_{\mathbf{J}}\varepsilon} \rangle$ is a U-statistic with square integrable kernel obtained from i.i.d. random vectors; it is thus asymptotically normal (Van der Vaart, 1998) and we simply need to compute its mean and variance. The mean is zero and a short calculation similar to the one found in the proof of Theorem 3 in Appendix B.2 shows that we have:

$$\begin{aligned} \mathbb{E}E_n^2 &\geq (1 - 1/n)\sigma_{\min}^2\langle v_i, \Sigma_{X_iX_i}v_i \rangle_{\mathcal{F}_i} + \sigma_{\min}^2\langle w_{\mathbf{J}}, \Sigma_{X_{\mathbf{J}}X_{\mathbf{J}}}w_{\mathbf{J}} \rangle_{\mathcal{F}_{\mathbf{J}}} - 2\sigma_{\min}^2\langle v_i, \Sigma_{X_iX_{\mathbf{J}}}w_{\mathbf{J}} \rangle_{\mathcal{F}_i} \\ &= (1 - 1/n)(\sigma_{\min}^2\langle v_i, \Sigma_{X_iX_i}v_i \rangle_{\mathcal{F}_i} - \sigma_{\min}^2\langle v_i, \Sigma_{X_iX_{\mathbf{J}}}w_{\mathbf{J}} \rangle_{\mathcal{F}_i}). \end{aligned}$$

The operator $C_{X_{\mathbf{J}}X_{\mathbf{J}}}^{-1}C_{X_{\mathbf{J}}X_i}$ has the same range as $C_{X_{\mathbf{J}}X_{\mathbf{J}}}$ (because $C_{X_{\mathbf{J}}X_{\mathbf{J}}}$ is invertible), and is thus included in the closure of the range of $\text{Diag}(\Sigma_{X_{\mathbf{J}}X_{\mathbf{J}}}^{1/2})$ (Baker, 1973). Thus, for any $u \in \mathcal{F}_i$, $C_{X_{\mathbf{J}}X_{\mathbf{J}}}^{-1}C_{X_{\mathbf{J}}X_i}u$ can be expressed as a limit of terms of the form $\text{Diag}(\Sigma_{X_{\mathbf{J}}X_{\mathbf{J}}}^{1/2})t$ where $t \in \mathcal{F}_{\mathbf{J}}$. We thus have that

$$\langle u, C_{X_iX_{\mathbf{J}}} \text{Diag}(\Sigma_{X_{\mathbf{J}}X_{\mathbf{J}}}^{1/2})w_{\mathbf{J}} \rangle_{\mathcal{F}_i} = \langle u, C_{X_iX_{\mathbf{J}}}C_{X_{\mathbf{J}}X_{\mathbf{J}}}^{-1}C_{X_{\mathbf{J}}X_{\mathbf{J}}} \text{Diag}(\Sigma_{X_{\mathbf{J}}X_{\mathbf{J}}}^{1/2})w_{\mathbf{J}} \rangle_{\mathcal{F}_i}$$

can be expressed as a limit of terms of the form

$$\begin{aligned} \langle t, \text{Diag}(\Sigma_{X_{\mathbf{J}}X_{\mathbf{J}}}^{1/2})C_{X_{\mathbf{J}}X_{\mathbf{J}}} \text{Diag}(\Sigma_{X_{\mathbf{J}}X_{\mathbf{J}}}^{1/2})w_{\mathbf{J}} \rangle_{\mathcal{F}_{\mathbf{J}}} &= \langle t, \Sigma_{X_{\mathbf{J}}X_{\mathbf{J}}}w_{\mathbf{J}} \rangle_{\mathcal{F}_{\mathbf{J}}} = \langle t, \Sigma_{X_{\mathbf{J}}X_i}v_i \rangle_{\mathcal{F}_{\mathbf{J}}} \\ &= \langle t, \text{Diag}(\Sigma_{X_{\mathbf{J}}X_{\mathbf{J}}}^{1/2})C_{X_{\mathbf{J}}X_i}\Sigma_{X_iX_i}^{1/2}v_i \rangle_{\mathcal{F}_{\mathbf{J}}} \rightarrow \langle u, C_{X_iX_{\mathbf{J}}}C_{X_{\mathbf{J}}X_{\mathbf{J}}}^{-1}C_{X_{\mathbf{J}}X_i}\Sigma_{X_iX_i}^{1/2}v_i \rangle_{\mathcal{F}_i}. \end{aligned}$$

This implies that $C_{X_iX_{\mathbf{J}}} \text{Diag}(\Sigma_{X_{\mathbf{J}}X_{\mathbf{J}}}^{1/2})w_{\mathbf{J}} = C_{X_iX_{\mathbf{J}}}C_{X_{\mathbf{J}}X_{\mathbf{J}}}^{-1}C_{X_{\mathbf{J}}X_i}\Sigma_{X_iX_i}^{1/2}v_i$, and thus we have:

$$\begin{aligned} \mathbb{E}E_n^2 &\geq \sigma_{\min}^2\langle v_i, \Sigma_{X_iX_i}v_i \rangle_{\mathcal{F}_i} - \sigma_{\min}^2\langle v_i, \Sigma_{X_iX_i}C_{X_iX_{\mathbf{J}}} \text{Diag}(\Sigma_{X_{\mathbf{J}}X_{\mathbf{J}}}^{1/2})w_{\mathbf{J}} \rangle_{\mathcal{F}_i} \\ &= \sigma_{\min}^2\langle v_i, \Sigma_{X_iX_i}v_i \rangle_{\mathcal{F}_i} - \sigma_{\min}^2\langle v_i, \Sigma_{X_iX_i}C_{X_iX_{\mathbf{J}}}C_{X_{\mathbf{J}}X_{\mathbf{J}}}^{-1}C_{X_{\mathbf{J}}X_i}\Sigma_{X_iX_i}^{1/2}v_i \rangle_{\mathcal{F}_i} \\ &= \sigma_{\min}^2\langle \Sigma_{X_iX_i}^{1/2}v_i, (I_{\mathcal{F}_i} - C_{X_iX_{\mathbf{J}}}C_{X_{\mathbf{J}}X_{\mathbf{J}}}^{-1}C_{X_{\mathbf{J}}X_i})\Sigma_{X_iX_i}^{1/2}v_i \rangle_{\mathcal{F}_i}. \end{aligned}$$

By assumption **(A5)**, the operator $I_{\mathcal{F}_i} - C_{X_iX_{\mathbf{J}}}C_{X_{\mathbf{J}}X_{\mathbf{J}}}^{-1}C_{X_{\mathbf{J}}X_i}$ is lower bounded by a strictly positive constant times the identity matrix, and thus, since $\Sigma_{X_iX_i}^{1/2}v_i \neq 0$, we have $\mathbb{E}E_n^2 > 0$. This implies that $n^{1/2}\langle v_i, \hat{\Sigma}_{X_iY} - \hat{\Sigma}_{X_iX_{\mathbf{J}}}\hat{f}_{\mathbf{J}} \rangle$ converges to a normal distribution with strictly positive variance. Thus the probability $\mathbb{P}\left(n^{1/2}\langle v_i, \hat{\Sigma}_{X_iY} - \hat{\Sigma}_{X_iX_{\mathbf{J}}}\hat{f}_{\mathbf{J}} \rangle_{\mathcal{F}_i} \geq d_i\|\hat{f}\|_d\|v_i\|_{\mathcal{F}_i} + 1\right)$ converges to a strictly positive limit (note that $\|\hat{f}\|_d$ can be replaced by $\|\mathbf{f}\|_d$ without changing the result). Since $\mu_n n^{1/2} \rightarrow \mu_0 < \infty$, this implies that

$$\mathbb{P}\left(\mu_n^{-1}\langle v_i, \hat{\Sigma}_{X_iY} - \hat{\Sigma}_{X_iX_{\mathbf{J}}}\hat{f}_{\mathbf{J}} \rangle_{\mathcal{F}_i} > d_i\|\hat{f}\|_d\|v_i\|_{\mathcal{F}_i}\right)$$

is asymptotically strictly positive (i.e., has a strictly positive lim inf). Thus the optimality condition (16) is not satisfied with non vanishing probability, which is a contradiction and proves the proposition. ■

We now go back to the proof of Theorem 12. We prove by contradiction, by assuming that there exists $i \in \mathbf{J}^c$ such that

$$\frac{1}{d_i} \left\| \Sigma_{X_iX_i}^{1/2} C_{X_iX_{\mathbf{J}}} C_{X_{\mathbf{J}}X_{\mathbf{J}}}^{-1} \text{Diag}(d_{\mathbf{J}}/\|\mathbf{f}_{\mathbf{J}}\|_{\mathcal{F}_{\mathbf{J}}}) \mathbf{g}_{\mathbf{J}} \right\|_{\mathcal{F}_i} > 1.$$

Since with probability tending to one $J(\hat{f}) = \mathbf{J}$, with probability tending to one, we have from optimality condition (17), and the usual line of arguments (see Eq. (41) in Appendix B.2) that for every $i \in \mathbf{J}^c$:

$$\begin{aligned}\hat{\Sigma}_{X_i Y} - \hat{\Sigma}_{X_i X_{\mathbf{J}}} \hat{f}_{\mathbf{J}} &= \mu_n \hat{\Sigma}_{X_i X_{\mathbf{J}}} \left(\hat{\Sigma}_{X_{\mathbf{J}} X_{\mathbf{J}}} + \mu_n D_n \right)^{-1} D_n \mathbf{f} \\ &\quad + \hat{\Sigma}_{X_i \varepsilon} - \hat{\Sigma}_{X_i X_{\mathbf{J}}} \left(\hat{\Sigma}_{X_{\mathbf{J}} X_{\mathbf{J}}} + \mu_n D_n \right)^{-1} \hat{\Sigma}_{X_{\mathbf{J}} \varepsilon},\end{aligned}$$

where $D_n = \|\hat{f}\|_d \text{Diag}(d_j / \|\hat{f}_j\|)$. Following the same argument as in the proof of Theorem 11, (and because $\mu_n n^{1/2} \rightarrow +\infty$ as a consequence of Proposition 26), the first term in the last expression (divided by μ_n) converges to

$$v_i = \Sigma_{X_i X_i}^{1/2} C_{X_i X_{\mathbf{J}}} C_{X_{\mathbf{J}} X_{\mathbf{J}}}^{-1} \|\mathbf{f}\|_d \text{Diag}(d_j / \|\mathbf{f}_j\|_{\mathcal{F}_j}) \mathbf{g}_{\mathbf{J}}$$

By assumption $\|v_i\| > d_i \|\mathbf{f}\|_d$. We have the second term:

$$\begin{aligned}&\hat{\Sigma}_{X_i \varepsilon} - \hat{\Sigma}_{X_i X_{\mathbf{J}}} \left(\hat{\Sigma}_{X_{\mathbf{J}} X_{\mathbf{J}}} + \mu_n \|\hat{f}\|_d \text{Diag}(d_j / \|\hat{f}_j\|_{\mathcal{F}_j}) \right)^{-1} \hat{\Sigma}_{X_{\mathbf{J}} \varepsilon} \\ &= O_p(n^{-1/2}) - \hat{\Sigma}_{X_i X_{\mathbf{J}}} \left(\hat{\Sigma}_{X_{\mathbf{J}} X_{\mathbf{J}}} + \mu_n \|\mathbf{f}\|_d \text{Diag}(d_j / \|\mathbf{f}_j\|_{\mathcal{F}_j}) \right)^{-1} \hat{\Sigma}_{X_{\mathbf{J}} \varepsilon} + O_p(n^{-1/2}).\end{aligned}$$

The remaining term can be bounded as follows (with $D = \|\mathbf{f}\|_d \text{Diag}(d_j / \|\mathbf{f}_j\|_{\mathcal{F}_j})$):

$$\begin{aligned}&\mathbb{E} \left(\left\| \hat{\Sigma}_{X_i X_{\mathbf{J}}} \left(\hat{\Sigma}_{X_{\mathbf{J}} X_{\mathbf{J}}} + \mu_n D \right)^{-1} \hat{\Sigma}_{X_{\mathbf{J}} \varepsilon} \right\|_{\mathcal{F}_i}^2 \mid \bar{X} \right) \\ &\leq \frac{\sigma_{\max}^2}{n} \text{tr} \hat{\Sigma}_{X_i X_{\mathbf{J}}} \left(\hat{\Sigma}_{X_{\mathbf{J}} X_{\mathbf{J}}} + \mu_n D \right)^{-1} \hat{\Sigma}_{X_{\mathbf{J}} X_{\mathbf{J}}} \left(\hat{\Sigma}_{X_{\mathbf{J}} X_{\mathbf{J}}} + \mu_n D \right)^{-1} \hat{\Sigma}_{X_{\mathbf{J}} X_i} \\ &\leq \frac{\sigma_{\max}^2}{n} \text{tr} \hat{\Sigma}_{X_i X_i},\end{aligned}$$

which implies that the full expectation is $O(n^{-1})$ (because our operators are trace-class, i.e., have finite trace). Thus the remaining term is $O_p(n^{-1/2})$ and thus negligible compared to μ_n , therefore $\frac{1}{\mu_n \|\hat{f}\|_d} \left(\hat{\Sigma}_{X_i Y} - \hat{\Sigma}_{X_i X_{\mathbf{J}}} \hat{f}_{\mathbf{J}} \right)$ converges in probability to a limit which is of norm strictly greater than d_i . Thus there is a non vanishing probability of being strictly larger than d_i , which implies that with non vanishing probability, the optimality condition (16) is not satisfied, which is a contradiction. This concludes the proof.

C.4 Proof of Proposition 15

Note that the estimator defined in Eq. (23) is exactly equal to

$$\left\| \hat{\Sigma}_{X_i X_{\mathbf{J}}} (\hat{\Sigma}_{X_{\mathbf{J}} X_{\mathbf{J}}} + \kappa_n I)^{-1} \text{Diag}(d_j / \|(\hat{f}_{\kappa_n}^{LS})_j\|_{\mathcal{F}_j}) (\hat{f}_{\kappa_n}^{LS})_{\mathbf{J}} \right\|_{\mathcal{F}_i}.$$

Using Proposition 17 and the arguments from Appendix C.2 by replacing \tilde{f} by \hat{F}_{LS} , we get the consistency result.

Appendix D. Proof of Results on Adaptive Group Lasso

D.1 Proof of Theorem 16

We define \tilde{w} as the minimizer of the same cost function restricted to $w_{\mathbf{J}^c} = 0$. Because \hat{w}^{LS} is consistent, the norms of \hat{w}_j^{LS} for $j \in \mathbf{J}$ are bounded away from zero, and we get from standard results on M-estimation (Van der Vaart, 1998) the normal limit distribution with given covariance matrix if $\mu_n \ll n^{-1/2}$.

Moreover, the patterns of zeros (which is obvious by construction of \tilde{w}) converges in probability. What remains to be shown is that with probability tending to one, \tilde{w} is optimal for the full problem. We just need to show that with probability tending to one, for all $i \in \mathbf{J}^c$,

$$\|\hat{\Sigma}_{X_i\varepsilon} - \hat{\Sigma}_{X_iX_{\mathbf{J}}}(\tilde{w}_{\mathbf{J}} - w_{\mathbf{J}})\| \leq \mu_n \|\tilde{w}\|_d \|\hat{w}_i^{LS}\|^{-\gamma}. \quad (42)$$

Note that $\|\tilde{w}\|_d$ converges in probability to $\|\mathbf{w}\|_d > 0$. Moreover, $\|\hat{w}_i^{LS} - \mathbf{w}_i\| = O_p(n^{-1/2})$. Thus, if $i \in \mathbf{J}^c$, i.e., if $\mathbf{f}_i = 0$, then $\|\hat{w}_i^{LS}\| = O_p(n^{-1/2})$. The left hand side in Eq. (42) is thus upper bounded by $O_p(n^{-1/2})$ while the right hand side is lower bounded asymptotically by $\mu_n n^{\gamma/2}$. Thus if $n^{-1/2} = o(\mu_n n^{\gamma/2})$, then with probability tending to one we get the correct optimality condition, which concludes the proof.

D.2 Proof of Proposition 17

We have:

$$\hat{f}_{\kappa_n}^{LS} = \left(\hat{\Sigma}_{XX} + \kappa_n I_{\mathcal{F}} \right)^{-1} \hat{\Sigma}_{XY},$$

and thus:

$$\begin{aligned} \hat{f}_{\kappa_n}^{LS} - \mathbf{f} &= \left(\hat{\Sigma}_{XX} + \kappa_n I_{\mathcal{F}} \right)^{-1} \hat{\Sigma}_{XX} \mathbf{f} - \mathbf{f} + \left(\hat{\Sigma}_{XX} + \kappa_n I_{\mathcal{F}} \right)^{-1} \hat{\Sigma}_{X\varepsilon} \\ &= (\Sigma_{XX} + \kappa_n I)^{-1} \Sigma_{XX} \mathbf{f} - \mathbf{f} + O_p(n^{-1/2} \kappa_n^{-1}) \text{ from Lemma 23} \\ &= -(\Sigma_{XX} + \kappa_n I_{\mathcal{F}})^{-1} \kappa_n \mathbf{f} + O_p(n^{-1/2} \kappa_n^{-1}). \end{aligned}$$

Since $\mathbf{f} = \Sigma_{XX}^{-1/2} \mathbf{g}$, we have $\| -(\Sigma_{XX} + \kappa_n I_{\mathcal{F}})^{-1} \kappa_n \mathbf{f} \|_{\mathcal{F}}^2 \leq C \kappa_n \|\mathbf{g}\|_{\mathcal{F}}^2$, which concludes the proof.

D.3 Proof of Theorem 18

We define \tilde{f} as the minimizer of the same cost function restricted to $f_{\mathbf{J}^c} = 0$. Because $\hat{f}_{n^{-1/3}}^{LS}$ is consistent, the norms of $(\hat{f}_{n^{-1/3}}^{LS})_j$ for $j \in \mathbf{J}$ are bounded away from zero, and Lemma 25 applies with $\mu_n = \mu_0 n^{-1/3}$, i.e., \tilde{f} converges in probability to \mathbf{f} and so are the patterns of zeros (which is obvious by construction of \tilde{f}). Moreover, for any $\eta > 0$, from Lemma 25, we have $\|\tilde{f}_{\mathbf{J}} - f_{\mathbf{J}}\| = O_p(n^{-1/6+\eta})$ (because $\mu_n^{-1/2} + n^{-1/2} \mu_n^{-1} = O_p(n^{-1/6})$).

What remains to be shown is that with probability tending to one, \tilde{f} is optimal for the full problem. We just need to show that with probability tending to one, for all $i \in \mathbf{J}^c$,

$$\|\hat{\Sigma}_{X_i\varepsilon} - \hat{\Sigma}_{X_iX_{\mathbf{J}}}(\tilde{f}_{\mathbf{J}} - f_{\mathbf{J}})\| \leq \mu_n \|\tilde{f}\|_d \|(\hat{f}_{n^{-1/3}}^{LS})_i\|_{\mathcal{F}_i}^{-\gamma}. \quad (43)$$

Note that $\|\tilde{f}\|_d$ converges in probability to $\|\mathbf{f}\|_d > 0$. Moreover, by Proposition 17, $\|(\hat{f}_{n^{-1/3}}^{LS})_i - \mathbf{f}_i\| = O_p(n^{-1/6})$. Thus, if $i \in \mathbf{J}^c$, i.e., if $\mathbf{f}_i = 0$, then $\|(\hat{f}_{n^{-1/3}}^{LS})_i\|_{\mathcal{F}_i} = O_p(n^{-1/6})$. The left hand

side in Eq. (43) is thus upper bounded by $O_p(n^{-1/2} + n^{-1/6+\eta})$ while the right hand side is lower bounded asymptotically by $n^{-1/3}n^{\gamma/6}$. Thus if $-1/6 + \eta < -1/3 + \gamma/6$, then with probability tending to one we get the correct optimality condition. As soon as $\gamma > 1$, we can find η small enough and strictly positive, which concludes the proof.

D.4 Range Condition of Covariance Operators

We let denote $C(q)$ the convolution operator by q on the space of real functions on \mathbb{R}^p and $T(p)$ the pointwise multiplication by $p(x)$. In this appendix, we look at different Hilbertian products of functions on \mathbb{R}^p , we use the notations $\langle \cdot, \cdot \rangle_{\mathcal{F}}$ and $\langle \cdot, \cdot \rangle_{L^2(p_X)}$ and $\langle \cdot, \cdot \rangle_{L^2(\mathbb{R}^p)}$ for the dot products in the RKHS \mathcal{F} , the space $L^2(p_X)$ of square integrable functions with respect to $p(x)dx$, and the space $L^2(\mathbb{R}^p)$ of square integrable functions with respect to the Lebesgue measure. With our assumptions, for all $\tilde{f}, \tilde{g} \in L^2(\mathbb{R}^p)$, we have:

$$\langle \tilde{f}, \tilde{g} \rangle_{L^2} = \langle C(q)^{1/2}\tilde{f}, C(q)^{1/2}\tilde{g} \rangle_{\mathcal{F}}.$$

Denote by $\{\lambda_k\}_{k \geq 1}$ and $\{e_k\}_{k \geq 1}$ the positive eigenvalues and the eigenvectors of the covariance operator Σ_{XX} , respectively. Note that since $p_X(x)$ was assumed to be strictly positive, all eigenvalues are strictly positive (the RKHS cannot contain any non zero constant functions on \mathbb{R}^p). For $k \geq 1$, set $f_k = \lambda_k^{-1/2}(e_k - \int_{\mathbb{R}^p} e_k(x)p_X(x)dx)$. By construction, for any $k, \ell \geq 1$,

$$\begin{aligned} \lambda_k \delta_{k,\ell} &= \langle e_k, \Sigma e_\ell \rangle_{\mathcal{F}} = \int_{\mathbb{R}^p} p_X(x)(e_k - \int_{\mathbb{R}^p} e_k(x)p_X(x)dx)(e_\ell - \int_{\mathbb{R}^p} e_\ell(x)p_X(x)dx)dx \\ &= \lambda_k^{1/2} \lambda_\ell^{1/2} \int_{\mathbb{R}^p} p_X(x) f_k(x) f_\ell(x) dx = \lambda_k^{1/2} \lambda_\ell^{1/2} \langle f_k, f_\ell \rangle_{L^2(p_X)}. \end{aligned}$$

Thus $\{f_k\}_{k \geq 1}$ is an orthonormal sequence in $L^2(p_X)$. Let $f = C(q)g$ for $g \in L^2(\mathbb{R}^p)$ such that $\int_{\mathbb{R}^p} g(x)dx = 0$. Note that f is in the range of $\Sigma_{XX}^{1/2}$ if and only if $\langle f, \Sigma^{-1}f \rangle_{\mathcal{F}}$ is finite. We have:

$$\begin{aligned} \langle f, \Sigma^{-1}f \rangle_{\mathcal{F}} &= \sum_{p=1}^{\infty} \lambda_p^{-1} \langle e_p, f \rangle_{\mathcal{F}}^2 = \sum_{p=1}^{\infty} \lambda_p^{-1} \langle e_p, g \rangle_{L^2(\mathbb{R}^p)}^2 = \sum_{p=1}^{\infty} \lambda_p^{-1} \left(\int_{\mathbb{R}^p} g(x) e_p(x) dx \right)^2 \\ &= \sum_{p=1}^{\infty} \langle p_X^{-1} g, f_p \rangle_{L^2(p_X)}^2 \leq \|p_X^{-1} g\|_{L^2(p_X)}^2 = \int_{\mathbb{R}^p} \frac{g^2(x)}{p_X(x)} dx, \end{aligned}$$

because $\{f_k\}_{k \geq 1}$ is an orthonormal sequence in $L^2(p_X)$. This concludes the proof.

Appendix E. Gaussian Kernels and Gaussian Variables

In this section, we consider $X \in \mathbb{R}^m$ with normal distribution with zero mean and covariance matrix S . We also consider Gaussian kernels $k_j(x_j, x'_j) = \exp(-b_i(x_j - x'_j)^2)$ on each of its component. In this situation, we can find orthonormal basis of the Hilbert spaces \mathcal{F}_j where we can compute the coordinates of all covariance operators. This thus allows to check conditions (18) or (19) without using sampling.

We consider the eigenbasis of the non centered covariance operators on each \mathcal{F}_j , $j = 1, \dots, m$, which is equal to (Zhu et al., 1998):

$$e_k^j(x_j) = (\lambda_k^j)^{1/2} \left(\frac{c_j^{1/2}}{a_j^{1/2} 2^k k!} \right)^{1/2} e^{-(c_j - a_j)u^2} H_k((2c_j)^{1/2} x_j)$$

with eigenvalues $\lambda_k^j = \left(\frac{2a_j}{A_j} \right)^{1/2} (B_j)^k$, where $a_i = 1/4 S_{ii}$, $c_j = (a_j^2 + 2a_j b_j)^{1/2}$, $A_j = a_j + b_j + c_j$ and $B_j = b_j/A_j$, and H_k is the k -th Hermite polynomial.

We can then compute all required expectations as follows (note that by definition we have $\mathbb{E} e_k^j(X_j)^2 = \lambda_k^j$):

$$\begin{aligned} \mathbb{E} e_{2k+1}^j(X_j) &= 0 \\ \mathbb{E} e_{2k}^j(X_j) &= \left(\lambda_{2k}^j \frac{2a_j^{1/2} c_j^{1/2}}{(a_j + c_j)} \binom{2k}{k} \right)^{1/2} \left(\frac{c_j - a_j}{2(c_j + a_j)} \right)^k \end{aligned}$$

$$\mathbb{E} e_k^j(X_j) e_\ell^i(X_i) = \left(\lambda_{2k}^j \lambda_{2\ell}^i \frac{c_j^{1/2} c_i^{1/2}}{a_j^{1/2} a_i^{1/2} 2^k 2^\ell k! \ell!} \right)^{1/2} \frac{(S_{ii} S_{jj} - S_{ij}^2)^{-1/2}}{4\pi c_i^{1/2} c_j^{1/2}} D_{k\ell}(Q_{ij}),$$

where $Q_{ij} = \begin{pmatrix} \frac{1}{2}(1 - a_i/c_i) & 0 \\ 0 & \frac{1}{2}(1 - a_j/c_j) \end{pmatrix} + \frac{1}{4} \begin{pmatrix} S_{ii} c_i & S_{ij} c_i^{1/2} c_j^{1/2} \\ S_{ij} c_i^{1/2} c_j^{1/2} & S_{jj} c_j \end{pmatrix}^{-1}$ and

$$D_{k\ell}(Q) = \int_{\mathbb{R}^2} \exp \left[- \begin{pmatrix} u \\ v \end{pmatrix}^\top Q \begin{pmatrix} u \\ v \end{pmatrix} \right] H_k(u) H_\ell(v) du dv,$$

for any positive matrix Q . For any given Q , $D_{k\ell}(Q)$ can be computed exactly by using a singular value decomposition of Q and the appropriate change of variables.⁵

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5. Matlab code to compute $D_{k\ell}(Q)$ can be downloaded from the author's webpage.

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