On the Self-Penalization Phenomenon in Feature Selection

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Abstract

We describe an implicit sparsity-inducing mechanism based on minimization over a family of kernels:

\[
\min_{\beta, f} \hat{E}[L(Y, f(\beta^{1/q} \odot X))] + \lambda_n \|f\|_{H_q}^2 \text{ subject to } \beta \geq 0,
\]

where \(L\) is the loss, \(\odot\) is coordinate-wise multiplication and \(H_q\) is the reproducing kernel Hilbert space based on the kernel \(k_q(x, x') = h(\|x - x'\|_q)\), where \(\|\cdot\|_q\) is the \(\ell_q\) norm.

Using gradient descent to optimize this objective with respect to \(\beta\) leads to exactly sparse stationary points with high probability. The sparsity is achieved without using any of the well-known explicit sparsification techniques such as penalization (e.g., \(\ell_1\)), early stopping or post-processing (e.g., clipping).

As an application, we use this sparsity-inducing mechanism to build algorithms consistent for feature selection.

Key Words. Kernel Regression. Sparsity. Self Penalization. Gradient Flow. Invariant Set.

1 Introduction

In supervised learning, we are given labeled data \((Y, X)\) and want to learn a function \(f(X)\) for predicting \(Y\). Whether motivated by domain knowledge or practical constraints, we may want the function \(f\) to depend on only a few of the features in \(X\). \(\ell_1\) regularization is the most well known mechanism for inducing sparsity in the components of \(X\). When \(f\) is assumed linear—\(f(x) = x^\top \beta\)—the Lasso objective uses squared loss and an \(\ell_1\) penalty on \(\beta\) to learn \(f\):

\[
\min_{\beta \in \mathbb{R}^p} \hat{E}[(Y - X^\top \beta)^2] + \gamma \|\beta\|_1,
\]

where \(\hat{E}\) is the empirical expectation over the data. The \(\ell_1\) penalty in the Lasso objective forces components of \(\beta\) to be exactly zero, operationalizing the notion of automatic selection of those features of \(X\) that are most relevant for predicting \(Y\).
This paper introduces a new sparsity-inducing mechanism which does not use any explicit $\ell_1$ penalty but still obtains sparsity in $f$. The mechanism relies on the fact that the stationary points of certain kernel-based empirical risk functions are naturally sparse with respect to the features—a fact that has not been previously noted. The usual kernel approach to learning $f$ solves the following optimization problem:

$$
\min_{f \in \mathcal{H}} \mathbb{E}[L(Y, f(X)) + \lambda_n \|f\|_{\mathcal{H}}^2],
$$

where $L$ is a loss function and $\mathcal{H}$ is a reproducing kernel Hilbert space (RKHS). The solution $f$ is generally not sparse in $X$. To induce sparsity, we consider a parametrized function, $f(\beta^{1/q} \odot X)$, where $\odot$ denotes coordinate-wise multiplication, and we simultaneously minimize the usual kernel objective over $f$ and $\beta$:

$$
\min_{\beta} F_n(\beta) \quad \text{subject to} \quad \beta \geq 0, \|\beta\|_{\infty} \leq M
$$

where $F_n(\beta) = \min_{f} \mathbb{E}[L(Y, f(\beta^{1/q} \odot X))] + \lambda_n \|f\|_{\mathcal{H}}^2$. We call $F_n(\beta)$ the kernel feature selection objective; in general, it is nonconvex in $\beta$. The ridge parameter $\lambda_n$ and the box constraint parameter $M$ are needed so that the solutions $(f, \beta)$ are bounded. Similar to the case of the Lasso, a feature $X_j$ is active in the learned prediction function if and only if $\beta_j \neq 0$; however, the kernel formulation lacks an explicit $\ell_1$ penalty for $\beta$ that aims to separate active from inactive features. Conventional wisdom suggests that we should not expect to obtain an exactly sparse solution $\beta$ by simply minimizing $F_n(\beta)$, at least not without some form of post-processing of the solution (e.g., clipping). Surprisingly, we observe many cases where the stationary points of the kernel feature selection objective are exactly sparse. We call this phenomenon self-penalization. The purpose of the paper is to (i) clarify the nature of self-penalization, and (ii) discuss its statistical consequences for (nonparametric) feature selection.

The phenomenon is present even in the restricted setting of kernel functions of the form $k(x, x') = h(||x - x'||_q^q)$, for $q \in \{1, 2\}$, and for simplicity our theoretical analysis will restrict attention to this setting. We further limit ourselves to two choices of the loss function $L$:

**Metric learning** Consider the classification setting where $X \in \mathbb{R}^p$ and $Y \in \{\pm 1\}$. Let $L$ be the margin-based loss $L(y, \hat{y}) = -y\hat{y}$. Then the objective has the following explicit form:

$$
F_n(\beta) = -\frac{1}{4\lambda_n} \mathbb{E}[YY' h(||X - X'||_q^q)],
$$

where $(X, Y)$ and $(X', Y')$ denote independent copies from the empirical distribution and $\|z\|_{q, \beta}$ denotes the weighted $\ell_q$ norm: $\|z\|_{q, \beta}^q = \sum_{i} \beta_i |z_i|^q$. We supply a short derivation of this result in Appendix F.2; see Liu and Ruan (2020) for a fuller presentation.

**Kernel ridge regression** Consider the regression setting where $X \in \mathbb{R}^p$ and $Y \in \mathbb{R}$. Let $L$ be the squared error loss $L(y, \hat{y}) = \frac{1}{2}(y - \hat{y})^2$. Define the objective function as follows:

$$
F_n(\beta) = \min_{f} \frac{1}{2} \mathbb{E}[(Y - f(\beta^{1/q} \odot X))^2] + \lambda_n \|f\|_{\mathcal{H}}^2.
$$


Both the metric learning and kernel ridge regression (KRR) objectives turn out to exhibit naturally sparse stationary points. To begin to study this phenomenon, let us consider a concrete example involving the metric learning objective. Suppose $X$ is uniformly distributed on the square $[-1, 1]^2$ and the response $Y \in \{\pm 1\}$ is balanced; i.e., $E[Y] = 0$. Let us assume that $E[Y|X] = X^3$. Figure 1 provides a graphical illustration of the gradient field of the empirical metric learning objective, equation (4), when $n = 20$. The figure clearly shows that despite the multiplicity of stationary points, the gradient flow, which moves along the negative gradient, converges to points that only select $X_1$.

Figure 1. The gradient field for the empirical metric learning objective (4). The sample size is $n = 20$ and the dimension is $p = 2$. The data as distributed according to $X_1, X_2 \sim \text{Unif}[-1, 1]$ and $E[Y|X] = X_1^3$. The arrows represent the negative gradients of the empirical metric learning objective.

The rest of the paper is organized as follows. Section 2 sets up the problem and introduces assumptions. Section 3 sketches the process by which self-penalizing objectives exclude noise variables. Section 4 supplies the formal definition of a self-penalizing objective and shows that the metric learning and kernel ridge regression objectives are self-penalizing while classical objectives, such as least squares, are not. Section 5 characterizes the behavior of gradient descent when applied to the metric learning and kernel ridge regression objectives: under appropriate conditions, gradient descent reaches sparse stationary points in finite time. Section 6 discusses how to use self-penalizing objectives to build consistent feature selection algorithms. Section 7 presents experiments to supplement our theory.

1.1 Notation

The notation $\mathbb{Q}$ is reserved for the population distribution of the data $(X, Y)$, and $\mathbb{Q}_n$ denotes the empirical distribution. The notation $\mathcal{H} \equiv \mathcal{H}_q$ stands for the $\ell_q$-type RKHS associated with the kernel function $k(x, x') = h(\|x - x'|^q_2)$.
Consider the following general kernel feature selection problem:

$$\min_{\beta} \quad F_\lambda(\beta; Q) \quad \text{subject to } \beta \geq 0, \|\beta\|_\infty \leq M.$$  \hspace{1cm} (6)

$$F_\lambda(\beta; Q) = \min_{f \in \mathcal{H}} \mathbb{E}_Q[L(Y, f(\beta^{1/q} \odot X))] + \frac{\lambda}{2} \|f\|_\mathcal{H}^2.$$  \hspace{1cm} (6)

When $Q = Q_n$ is the empirical distribution over data $(X_i, Y_i)$, $F_\lambda(\beta; Q_n)$ is the empirical kernel feature selection objective; setting $Q$ as the population distribution of $(X, Y)$ yields the population objective. $\beta$ enters the objective in the form $\beta^{1/q}$, which takes on one of two values depending on the choice of $q \in \{1, 2\}$ in the kernel $k(x, x') = h(\|x - x'\|_q^q)$.

This paper considers using projected gradient descent to solve the nonconvex problem (6) and focuses on describing the sparsity pattern of the solutions. Let $\mathcal{B} = \{\beta : \beta \geq 0, \|\beta\|_\infty \leq M\}$ be the feasible set (which is convex). We consider the projected gradient descent algorithm:

$$\beta(k + 1) = \Pi_\mathcal{B}(\beta(k) - \alpha \nabla F_\lambda(\beta(k); Q)) \quad \text{for } k = 0, 1, 2, \ldots,$$  \hspace{1cm} (7)

where $\Pi_\mathcal{B}$ denotes the $\ell_2$ projection onto the set $\mathcal{B}$; i.e., $\Pi_\mathcal{B}(z) = \arg\min_{\beta \in \mathcal{B}} \|\beta - z\|_2$. To simplify the analysis, we also consider the projected gradient inclusion, which is, intuitively speaking, the limit of the projected gradient iterates after taking the stepsize $\alpha \to 0^+$, and is defined as follows:

$$\dot{\beta}(t) \in -\nabla F_\lambda(\beta(t); Q) - N_\mathcal{B}(\beta(t)), \quad \text{and } \beta(0) \in \mathcal{B},$$  \hspace{1cm} (8)

where $N_\mathcal{B}$ denotes the normal cone with respect to the convex set $\mathcal{B}$. Appendix B presents a formal treatment of the projected gradient inclusion [5], showing that the solution $t \mapsto \beta(t)$ exists whenever $\beta \mapsto \nabla F_\lambda(\beta; \mathcal{P})$ is Lipschitz in the feasible set $\mathcal{B}$.

Two special cases of the general kernel feature selection objective are of interest to us: the metric learning objective in [4] and the kernel ridge regression objective in [5]. We reproduce them here using our formal notation:

$$F_{\text{ML}}(\beta; Q) = -\mathbb{E}_Q[YY'h(\|X - X'\|_{q, \beta}^q)]$$  \hspace{1cm} (9)
\[
F^KRR(\beta; \mathcal{Q}) = \min_{f \in \mathcal{H}} \frac{1}{2} \mathbb{E}_\mathcal{Q}[(Y - f(\beta^{1/q} \odot X))^2] + \frac{\lambda}{2} \|f\|^2_H.
\] (10)

Since both the metric learning and kernel ridge regression objectives are smooth in \(\beta\), the projected gradient descent inclusion is well defined for any probability measure \(\mathcal{Q}\).

Our results are based on two technical assumptions. The first assumption is concerned with the regularity of the RKHS \(\mathcal{H}\). Recall that \(\mathcal{H}\) is the RKHS associated with a kernel of the form \(h(\|x - x'\|^q)\) where \(q \in \{1, 2\}\). According to Bernstein’s theorem (see, e.g., Ruan et al. 2021, Proposition 1), for either \(q = 1\) or \(q = 2\), there exists an RKHS \(\mathcal{H}\) corresponding to a function \(h \in C^\infty(\mathbb{R}^+)\) if and only if the function \(h\) satisfies the following:

\[
h(z) = \int_0^\infty e^{-tz} \mu(dt),
\] (11)

for some measure \(\mu\) on \(\mathbb{R}^+\) with \(\mu((0, \infty)) > 0\). Let \(m_\mu = \inf\{x : x \in \text{supp}(\mu)\}\) and \(M_\mu = \sup\{x : x \in \text{supp}(\mu)\}\).

**Assumption 1.** Assume that \(\text{supp}(\mu)\) is bounded and bounded away from zero: \(0 < m_\mu < M_\mu < \infty\).

**Remark** Assumption \(\square\) can be easily verified using the following equivalent characterization: (i) the function \(h \in C^\infty(\mathbb{R}^+)\) is completely monotone, i.e., \((-1)^k h^{(k)}(x) > 0\) for all \(k \in \mathbb{N}\), and (ii) the function \(h'(z)\) has exponential decay: \(C_1 e^{-c_1 z} \leq h'(z) \leq C_2 e^{-c_2 z}\) holds for all \(z \in \mathbb{R}^+\), where \(C_1, C_2, c_1, c_2\) are independent constants. Assumption \(\square\) holds for a range of functions including the important case of \(h(z) = \exp(-z)\).

Our second assumption concerns the regularity of the population distribution \(\mathcal{Q}\).

**Assumption 2.** Assume the distribution \(\mathcal{Q}\) has the following properties:

(i) The response \(Y\) is centered: \(\mathbb{E}_\mathcal{Q}[Y] = 0\).

(ii) The support of \((X, Y)\) is bounded under \(\mathcal{Q}\): \(\|X\|_\infty \leq M_X < \infty, |Y| \leq M_Y < \infty\).

(iii) The coordinates of \(X\) have non-vanishing variance: \(\text{Var}_\mathcal{Q}(X_l) > 0\) for all \(l \in [p]\).

**Remark** Assumption (i) is simply for convenience; we can dispense with it by adding an intercept to the objective—the new objective with the intercept would inherit all of the properties stated in the paper. Assumption (ii) is also imposed to simplify the exposition and can be replaced by a weaker assumption; e.g., a sub-gaussian assumption. In our proofs, it is mainly used to guarantee that population and empirical quantities (objective values and gradients) are uniformly close to each other.

### 3 Main Results

In this section we present our main result: that projected gradient descent (or gradient inclusion) applied to the metric learning or kernel ridge regression objectives induces exactly sparse solutions in finite samples with high probability. This result holds without any use of explicit regularization techniques such as \(\ell_1\) regularization or early stopping.
A necessary condition for a sparsity-inducing mechanism to arise is that there is some form of constraint on the dependence structure of the features. Indeed, consider the extreme case in which all of the covariates are all equal: \(X_1 = X_2 = \ldots = X_p\). If the initialization has equal coordinates, \(\beta_1(0) = \ldots = \beta_p(0)\), then the population gradient flow, by symmetry, must have equal coordinates along the entire trajectory. Consequently, the gradient flow can’t converge to a sparse solution (with the exception of \(\beta = 0\)). With this counterexample in mind, we divide the total set of indices, \(\{1, \ldots, p\}\), into complementary subsets, \(S\) and \(S^c\), such that a variable is in \(S\) if it is either indispensable for predicting \(Y\) (in the sense that we can’t achieve perfect prediction without this variable) or it is highly correlated with a variable that is indispensable for predicting \(Y\). Our results will show that projected gradient descent converges to a point whose support is contained in \(S\). We begin by presenting a formal definition of \(S\).

**Definition 3.1 (Signal Set \(S\) and Noise Set \(S^c\)).** The signal set \(S\) with respect to a measure \(Q\) is defined as the minimal subset \(S \subseteq \{p\}\) such that the following holds:

- \(\mathbb{E}_Q[Y|X] = \mathbb{E}_Q[Y|X_S]\); i.e., the signal \(X_S\) has full predictive power for \(Y\) given \(X\).
- \(X_S \perp X_{S^c}\) under \(Q\); i.e., the noise variables are independent of the signal variables.

Such a minimal set \(S\) is unique and always exists [Ruan et al., 2021, Proposition 16].

The set \(S\) represents an upper bound on the set of variables that are chosen via kernel feature selection. This upper bound \(S\) may be loose in terms of describing the variables actually chosen, but it describes the limit of what we are able to prove. As a concrete illustration, consider a simple case in which there are two dependent but non-equal covariates, \(X = (X_1, X_2)\), for which \(\mathbb{E}_Q[Y|X] = \mathbb{E}_Q[Y|X_1]\). In this case, \(S = \{1, 2\}\) (by definition) so our results cannot preclude the possibility that gradient descent converges to a point where \(\beta_2 > 0\). (It is difficult, however, to construct a numerical counterexample in which \(\beta_2 > 0\); see further discussion in Section 7). As a consequence, the characterization of the self-regularization phenomenon that we give in Theorems 1A and 1B is most accurate when signal and noise variables are not highly correlated. When significant correlation exists, kernel feature selection continues to deliver sparse solutions but our theoretical understanding in these situations is limited.

**Theorem 1A.** Given Assumptions 1 and 2, assume that the set of signals is not empty: \(S \neq \emptyset\). Consider the trajectory \(t \mapsto \tilde{\beta}(t)\) of the gradient flow with respect to the empirical metric learning objective \(F_{\text{ML}}(:, Q_n)\). Choose the initialization to be of full support: \(\text{supp}(\tilde{\beta}(0)) = [p]\). Then, with probability at least \(1 - e^{-cn}\), we have:

\[
\emptyset \neq \text{supp}(\tilde{\beta}(t)) \subseteq S \quad \text{holds for all } t \geq \tau,
\]

where the constants \(c, \tau > 0\) are independent of the sample size \(n\).

**Remark** The independence assumption \(X_S \perp X_{S^c}\) can be relaxed. Instead we can assume \(g(X_S, X_{S^c}) < \vartheta \cdot |F(\tilde{\beta}(0); Q)|\) for a constant \(\vartheta > 0\) that depends only on \(M_X, M_Y\) and \(\mu\) (and not on \(n\)). Here \(g(X_S, X_{S^c})\) is the maximal correlation between \(X_S\) and \(X_{S^c}\) (Rényi, 1959). See Appendix F for details.

Theorem 1B shows that the gradient flow of the kernel ridge regression objective also produces sparse solutions.
Theorem 1B. Given Assumptions 1 and 2, assume that the set of main effect signals is not empty $\hat{S} = \{ l \in S : \text{Var}_Q(\mathbb{E}_Q[Y|X_l]) \neq 0 \} \neq \emptyset$. Consider the trajectory $t \mapsto \tilde{\beta}(t)$ of the gradient flow with respect to the empirical kernel ridge regression objective $F_{\text{KRR}}^\lambda(\cdot; Q_n)$. Choose the initialization to be $\beta(0) = 0$. Set the parameter $q = 1$. There exists a constant $\lambda_0 > 0$ such that whenever $\lambda_n \leq \lambda_0$, we have, with probability at least $1 - e^{-cn\lambda_0^2}$,

$$\emptyset \neq \text{supp}(\tilde{\beta}(t)) \subseteq S \text{ holds for all } t \geq \tau,$$

where the constants $\lambda_0, c, \tau$ are independent of the sample size $n$.

Remark. Theorem 1B requires slightly more stringent conditions than Theorem 1A: (i) the existence of the “main effect” signals; i.e., $\mathbb{E}_Q[Y|X_l] \neq \mathbb{E}_Q[Y]$ where $l \in S$ and (ii) $q = 1$. These assumptions are very likely artifacts of the proof. In fact, our numerical experiments demonstrate that as long as $S \neq \emptyset$, with initialization $\beta(0)$ of full support, the gradient flow of the kernel ridge regression objective produces sparse solutions for both $q = 1$ and $q = 2$. In particular, if $Y$ and $X$ are related through pure interactions, the solutions are sparse (Section 7). Additionally, our experiments show that the assumption $X_S \perp X_{S^c}$ can be weakened to allow weak dependence.

Theorem 1A and 1B describe cases where running gradient descent on the metric learning or KRR objective produces solutions that include at least one signal variable and exclude all noise variables. This intriguing property enhances the further development of algorithms that are selection consistent; i.e., outputs $\hat{S}$ of an algorithm satisfy $\hat{S} \subseteq S$ and $\mathbb{E}[Y|X] = \mathbb{E}[Y|X_{\hat{S}}]$. Essentially, this is achieved by running gradient descent multiple times on a carefully constructed sequence of ML or KRR objectives; see Section 6.

3.1 Proof outline

In this section we provide a sketch of the main ideas underlying the proofs of Theorem 1A and Theorem 1B with the details deferred to Sections 4 and 5.

We use $F(\beta; Q)$ and $F(\beta; Q_n)$ to denote the population and empirical objectives, and let $t \mapsto \beta(t)$ and $t \mapsto \tilde{\beta}(t)$ denote the trajectories of the gradient flow with respect to the population and empirical objectives.

Our first goal is to show that the population dynamics satisfy $\emptyset \subseteq \text{supp}(\beta(t)) \subseteq S$ for all $t \geq \tau$ for some $\tau < \infty$. The key is to construct a subset $B \subseteq S$ such that (i) $0 \notin B$, and (ii) the population objective and its associated gradient flow satisfy the following properties:

- The gradient flow enters $B$ in finite time; i.e., $\beta(t_0) \in B$ for some $t_0 < \infty$.
- The set $B$ is invariant with respect to the gradient flow—any trajectory $t \mapsto \beta(t)$ entering the set $B$ will remain in the set $B$ ([Hale and Koçak, 2012]).
- The objective $F(\beta; Q)$ is self-penalizing on the set $B$—the gradients with respect to the noise variables when restricting to $\beta \in B$ are uniformly lower bounded away from zero:

$$\min_{\beta \in B} \inf_{\beta, \beta \in B} \partial_{\beta} F(\beta; Q) \geq c > 0. \quad (14)$$
The first two properties imply that after time $t_0$, we have $\beta(t) \in B$ for $t > t_0$. The self-penalizing property in Eq. (14) tells us that, since $\beta(t) \in B$, the coordinates corresponding to noise variables, $\beta_j(t)$ for $j \in S^c$, are either zero or are strictly decreasing at a positive rate. The net result of all three properties is that for some $\tau < \infty$, the dynamics must satisfy $\emptyset \subseteq \text{supp}(\beta(t)) \subseteq S$ for all $t \geq \tau$ (NB: $\beta(t) \neq 0$ since $0 \notin B$).

![Gradient Flow](image)

**Figure 2.** A pictorial illustration of the proof idea. In the example, $\beta_1$ (x-axis) corresponds to the signal variable, and $\beta_2$ (y-axis) corresponds to the noise variable. We use the shaded area to represent the specific set $B$ (or $B_n$) used in the proof. The proof logic is as follows: The gradient flow (i) enters $B$ in finite time, (ii) stays in $B$ once it enters (i.e., $B$ is an invariant set), and (iii) drives the noise variable $\beta_2$ to exactly zero in finite time as the objective is self-penalizing on the set $B$ (i.e., the gradient of the objective with respect to the noise variable $\beta_2$ is strictly positive, and in fact, bounded away from zero on the set $B$).

Next, we want to prove a similar result for the empirical dynamics $t \mapsto \tilde{\beta}(t)$. To do so, we will construct a set $B_n \subseteq B$, and a high probability event $\Omega_n$ such that on the event $\Omega_n$, the empirical objective and its gradient flow satisfy

- The empirical gradient dynamics enters $B_n$ in finite time: $\tilde{\beta}(t_0) \in B_n$ where $t_0 < \infty$.
- The set $B_n$ is invariant with respect to the empirical gradient flow—any trajectory $t \mapsto \tilde{\beta}(t)$ entering the set $B_n$ would remain in the set $B_n$ afterwards.
- The objective $F(\beta; Q_n)$ is self-penalizing on the set $B_n$:

$$\min_{j \notin S} \inf_{\beta : \beta \in B_n} \partial_{\beta_j} F(\beta; Q_n) \geq c/2 > 0. \quad (15)$$
By the same reasoning as above, it follows that for some \( \tau < \infty \), the empirical dynamics satisfy \( \emptyset \subsetneq \text{supp}(\hat{\beta}(t)) \subseteq S \) on the event \( \Omega_n \) for all \( t \geq \tau \).

Formally, \( \Omega_n \) is defined as the event where the objective values and the gradients of the population and empirical objectives are uniformly close (up to some \( \epsilon_n \) where \( \epsilon_n \to 0 \)) on the feasible set \( \mathcal{B} \). Defining \( \Omega_n \) in this way immediately yields that the self-penalizing property of the empirical objective in Eq. (15) is directly inherited from that of the population objective.

The construction of the sets \( \mathcal{B} \) and \( \mathcal{B}_n \) is trickier. A key idea is to utilize the fact that the sublevel sets of the minimizing objective, no matter whether it is a population or an empirical objective, are always an invariant set with respect to the corresponding gradient dynamics. The specific details of \( \mathcal{B} \) and \( \mathcal{B}_n \) will depend on the particular structure of the metric learning and KRR objectives; see Section 5.

### 4 The Notion of Self-Penalization

This section provides a general treatment of self-penalization. Section 4.1 introduces the formal definition of self-penalization. Section 4.2 shows that the linear-type objectives—which include classical least square objectives and nonnegative garrottes—are not self-penalizing objectives, even if their \( \ell_1 \) penalized versions are. This explains the necessity of using explicit \( \ell_1 \) regularization to attain sparse solutions for linear-type objectives. Section 4.3 and Section 4.4 show that, in contrast to the linear objectives, the two kernel-based feature selection objectives, namely, the metric learning and the kernel ridge regression objectives, are self-penalizing objectives. This has significant statistical implications: the nonlinear-type objectives—which model the prediction function using RKHS with \( \ell_q \)-type kernels in formulation (6)—are able to exclude noise variables even without the aid of \( \ell_1 \) regularization. The implications of these results to feature selection will be deferred to Section 6.

#### 4.1 Formal definition

This section formalizes the concept of self-penalization. Recall the definition of the signal set \( S \), which is defined as the minimal subset of \( \{1, 2, \ldots, p\} \) such that (i) \( \mathbb{E}_Q[Y|X] = \mathbb{E}_Q[Y|X_S] \) and (ii) \( X_S \perp X_{S^c} \) under \( Q \). The set of noise variables is the complement set \( S^c \).

We consider the minimization problem \( \min_{\beta \in \mathcal{B}} F(\beta; Q) \) where \( \mathcal{B} \) is a convex constraint set. The variable \( \beta \in \mathbb{R}^p \) is a \( p \)-vector whose coordinate is associated with the feature \( X \) in a way that \( \beta_j > 0 \) if and only if \( X_j \) is active. Assume \( \beta \mapsto F(\beta; Q) \) is locally Lipschitz.

**Definition 4.1.** A minimizing objective \( F(\beta; Q) \) is self-penalizing with respect to a relatively open subset \( \mathcal{B} \subseteq \mathcal{B} \) if (i) the objective \( F(\beta; Q) \) is differentiable on a set \( \mathcal{B}^0 \) dense in \( \mathcal{B} \) with the property that the gradient with respect to noise variables are bounded away from zero:

\[
\min_{\beta \in \mathcal{B}} \inf_{\beta \in \mathcal{B}^0} \sum_{j \notin S} \text{sign}(\beta_j) \cdot \partial_{\beta_j} F(\beta; Q) > 0, \tag{16}
\]

(ii) \( \mathcal{B} \) intersects non-trivially with the set of stationary points with no false positives. Formally, \( \mathcal{B} \cap \{ \beta \in \mathcal{B}^*: \text{supp}(\beta) \subseteq S \} \neq \emptyset \) where \( \mathcal{B}^* = \{ \beta \in \mathcal{B}: 0 \in \partial F(\beta; Q) + N_\mathcal{B}(\beta) \} \) denotes...
the set of Clarke stationary points. Here $\partial F(\beta; Q)$ denotes the Clarke subdifferential of $F$ and $N_B(\beta)$ denotes the normal cone of $B$ at $\beta$. 

As discussed in Section 3.1, Definition 4.1 is particularly useful when the set $B$ is invariant with respect to the gradient flow associated with the objective; i.e., once the gradient flow enters $B$, it never leaves. In that case, with the assumption that the gradient descent enters $B$, the gradient flow $\beta(t)$ must satisfy $\text{supp}(\beta(t)) \subseteq S$ for all (sufficiently) large $t$. This follows from the fact that the coefficients for the noise variables are guaranteed to approach zero at a strictly positive rate once the gradient flow enters $B$; see Eq. (16).

4.2 Linear-type objectives fail to be self-penalizing

This section shows that many linear-type objectives, i.e., those which model the prediction function as linear in the features, are not self-penalizing. Without loss of generality we assume throughout this section that both the features and the response are centered, i.e., $E_Q[X] = 0$ and $E_Q[Y] = 0$.

Example 1 (Ordinary Least Squares/Lasso (Tibshirani, 1996)): The Lasso (without intercept) is

$$
\min_{\beta: \beta \in \mathbb{R}^p} F_{\text{OLS}}(\beta; Q) \text{ where } F_{\text{OLS}}(\beta; Q) = \frac{1}{2} E_Q[(Y - \sum_{i=1}^p \beta_i X_i)^2] + \gamma \|\beta\|_1.
$$

The coefficient $\gamma \geq 0$ is known as the $\ell_1$ regularization parameter.

Example 2 (Nonnegative Garrotte (Breiman, 1995)): The nonnegative garrotte is a two stage procedure. In the first stage, it computes the ordinary least squares estimator, $w \in \mathbb{R}^p$, of $Y$ on $X$ under $Q$. In the second stage, it performs the following minimization

$$
\min_{\beta: \beta \in \mathbb{R}_+^p} F_{\text{NG}}(\beta; Q) \text{ where } F_{\text{NG}}(\beta; Q) = \frac{1}{2} E_Q[(Y - \sum_{i=1}^p \beta_i w_i X_i)^2] + \gamma \sum_{i=1}^p \beta_i.
$$

The procedure treats $X_j$ active if and only if $\beta_j > 0$.

For later comparison to nonlinear objectives, we give an additional example in which the objective has the same form as the kernel feature objective in Eq. (6), but it is based on a linear kernel.

Example 3 (Linear Kernel Objective): We consider the following procedure:

$$
\min_{\beta: \beta \in \mathbb{R}_+^p} F_{\text{LIN}}(\beta; Q) \text{ where } F_{\text{LIN}}(\beta; Q) = \min_w \frac{1}{2} E_Q[(Y - \sum_{i=1}^p \beta_i w_i X_i)^2] + \lambda \|w\|_2^2.
$$

An equivalent way to write $F_{\text{LIN}}$ is (cf. Eq. (6)):

$$
F_{\text{LIN}}(\beta; Q) = \min_{f \in \mathcal{H}} \frac{1}{2} E_Q[(Y - f(\beta \odot X))^2] + \lambda \|f\|_{\mathcal{H}}^2,
$$

\(^1\)We restrict attention to the case where the objective $\beta \mapsto F(\beta; Q)$ is either continuously differentiable or convex (which can be nonsmooth). The Clarke subdifferential $\partial F(\beta; Q)$ is the gradient when $F$ is continuously differentiable, and the set of subgradients when $F$ is convex (Rockafellar and Wets, 2009).
where $\mathcal{H}$ is the RKHS associated with the linear kernel, $k(x, x') = \langle x, x' \rangle$. We also define its $\ell_1$-penalized version: $F_{\lambda,\gamma}^\text{LIN}(\beta; \mathcal{Q}) = F_{\lambda}^\text{LIN}(\beta; \mathcal{Q}) + \gamma \sum_i \beta_i$. ♣

The following propositions show that these linear-type objectives are not self-penalizing, no matter how the set $B$ is chosen in the Definition 4.1. The proofs for Propositions 1B and 1C are deferred to Appendix C.2 and Appendix C.3 respectively.

**Proposition 1A.** The objective $F_{\gamma}^\text{OLS}(\beta; \mathcal{Q})$ is self-penalizing if and only if $\gamma > 0$.

**Proof** No matter how $B$ is defined, it must intersect non-trivially with $B^*$ (Definition 4.1); hence, to prove that $F_{\gamma}^\text{OLS}$ cannot be self-penalizing it suffices to show that the property in equation (16) cannot hold for points near $B^*$. In this case, the set of stationary points $B^*$ consists only of the set of global minima since the Lasso objective is convex.

Denote $B^0 = \{ \beta \in \mathbb{R}^p : \beta_i \neq 0 \text{ for } i \in [p] \}$, the set where the objective is differentiable. Fix a noise variable $j \notin S$. We show that for any $\beta^* \in B^*$,

$$\lim_{\beta \to \beta^*, \beta \in B^0} \frac{\partial}{\partial \beta_j} F_{\gamma}^\text{OLS}(\beta; \mathcal{Q}) = \gamma \text{.} \quad (17)$$

Denote $r_\beta(X; Y) = Y - \sum_{i=1}^p \beta_i X_i$ as the residual. At any $\beta \in B^0$,

$$\frac{\partial}{\partial \beta_j} F_{\gamma}^\text{OLS}(\beta; \mathcal{Q}) = \gamma - \text{sign}(\beta_j) \cdot \mathbb{E}_Q \left[ X_j r_\beta(X; Y) \right] \quad (18)$$

Note $\lim_{\beta \to \beta^*} \mathbb{E}_Q [X_j r_\beta(X; Y)] = \mathbb{E}_Q [X_j r_{\beta^*}(X; Y)] = \text{Cov}_Q (X_j, r_{\beta^*}(X; Y)) = 0$ where the second identity uses (i) $\text{supp}(\beta^*) \subseteq S$, (ii) $\mathbb{E}[Y|X] = \mathbb{E}[Y|X_S]$ and (iii) $X_S \perp X_{S^c}$. □

**Proposition 1B.** The objective $F_{\gamma}^\text{NG}(\beta; \mathcal{Q})$ is self-penalizing if and only if $\gamma > 0$.

**Proposition 1C.** The objective $F_{\lambda,\gamma}^\text{LIN}(\beta; \mathcal{Q})$ is self-penalizing if and only if $\gamma > 0$.

### 4.3 Metric learning is self-penalizing

This section shows that the metric learning objective $F_{\lambda}^\text{ML}(\beta; \mathcal{Q})$ is a self-penalizing objective. Remarkably, there is no explicit $\ell_1$ regularization in the definition of $F_{\lambda}^\text{ML}(\beta; \mathcal{Q})$. Recall the metric learning objective (see Eq. (9)):

$$F_{\lambda}^\text{ML}(\beta; \mathcal{Q}) = -\mathbb{E}[Y y'h(\|X - X'\|^2_{q,\beta})] \quad (19)$$

Importantly, the metric learning objective $F_{\lambda}^\text{ML}(\beta; \mathcal{Q})$ is a nonparametric dependence measure (see [Liu and Ruan, 2020], Proposition 3).

**Proposition 2.** Assume $\mathbb{E}_Q[Y] = 0$. Then the metric learning objective $F_{\lambda}^\text{ML}(\beta; \mathcal{Q})$ is a nonparametric dependence measure with the following properties:

- **Negativeness:** $F(\beta; \mathcal{Q}) \leq 0$ for all $\beta \geq 0$
- **Strict negativeness:** $F(\beta; \mathcal{Q}) < 0$ if and only if $Y \not\perp X_{\text{supp}(\beta)}$ under $\mathcal{Q}$. 

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We show that the metric learning objective is self-penalizing as long as the signal set $S$ is not empty. The core technical argument is the following lower bound on the gradient with respect to the noise variables. The proof is given in Section 4.5.

**Theorem 2.** Given Assumptions 1 and 2, the following holds for all $\beta \geq 0$ and $j \notin S$:

$$\partial_{\beta_j} F_{\text{ML}}(\beta; Q) \geq c(\beta) \cdot |F_{\text{ML}}(\beta; Q)|.$$  \hspace{1cm} (20)

Above $c(\beta) := m_{\mu} \cdot Ex_{q}[e^{-M_{\mu} \|X_{Sc} - X'_{Sc}\|_q} \cdot |X_j - X'_j|^q]$ is continuous and strictly positive. In particular, $\inf_{\beta \in B} c(\beta) = c > 0$ where $B = \{\beta : \beta \geq 0, \|\beta\|_{\infty} \leq M\}$ is the feasible set.

**Remark**  Theorem 2 shows that the gradient with respect to the noise variables is lower bounded by the objective value itself (up to a constant), and the objective value is a quantitative measure of the dependence between $Y$ and $X_{\text{supp}(\beta)}$. This is a general characteristic of kernel-based objectives—the strength of self-penalization (measured by the lower bound of the gradient with respect to noise) is dependent on the predictive power of the selected variables.

Theorem 2 immediately implies that the metric learning objective is self-penalizing.

**Corollary 4.1.** Given Assumptions 1 and 2 assume $S \neq \emptyset$. Let $B$ denote the feasible set. Define for any $c > 0$ the following set (which is relatively open with respect to $B$):

$$B_c = \{\beta \in B : |F_{\text{ML}}(\beta; Q)| > c\}.$$  \hspace{1cm}

Then (i) the set $B_c \neq \emptyset$ for small enough $c > 0$, and (ii) $F_{\text{ML}}(\beta; Q)$ is self-penalizing with respect to the set $B_c$ whenever $B_c \neq \emptyset$ and $c > 0$.

**Proof**  As $F_{\text{ML}}(\beta; Q)$ is a nonparametric dependence measure, $|F_{\text{ML}}(\beta; Q)| > 0$ as long as $S \subseteq \text{supp}(\beta)$ (Proposition 2). This proves that $X_c \neq \emptyset$ for small enough $c > 0$. The rest of the corollary follows from the gradient lower bound (Eq. (20)) in Theorem 2. \hfill $\blacksquare$

### 4.4 Kernel ridge regression is self-penalizing

This section shows that the kernel ridge regression objective $F_{\text{KRR}}^{\lambda}(\beta; Q)$ is a self-penalizing objective. We define the kernel ridge regression objective as follows (Ruan et al., 2021):

$$F_{\lambda}^{\text{KRR}}(\beta; Q) = \min_{f \in H} \frac{1}{2} Ex[(Y - f(\beta^{1/q} \circ X))^2] + \frac{\lambda}{2} \|f\|^2_H.$$  \hspace{1cm} (21)

Intuitively, the kernel ridge regression objective $F_{\lambda}^{\text{KRR}}(\beta; Q)$ is a proxy for the unexplained variance of $Y$ given $X_{\text{supp}(\beta)}$ (if the RKHS $H$ is universal; see Micchelli et al. (2006) for the definition). We have the following result, whose proof is given in Section C.4.

**Proposition 3.** Given Assumption 4 the following limit holds for any $\beta \geq 0$ for the RKHS $H$ whose associated kernel is of the form $h(||x - x'||_q^q)$, where $q \in \{1, 2\}$:

$$\lim_{\lambda \to 0^+} F_{\lambda}^{\text{KRR}}(\beta; Q) = \frac{1}{2} \cdot Ex[\text{Var}(Y|X_{\text{supp}(\beta)})].$$  \hspace{1cm} (22)
We show that the KRR objective is self-penalizing as long as the signal set is not empty. The core technical argument is the gradient lower bound which we provide in the following theorem whose proof is given in Section 4.6.

**Theorem 3.** Given Assumptions 1 and 2, the following holds for all \( \beta \geq 0 \) and \( j \not\in S \):

\[
\partial_{\beta_j} F^\text{KRR}_\lambda(\beta; \mathbb{Q}) \geq c_j \cdot \lambda (F^\text{KRR}_\lambda(0; \mathbb{Q}) - F^\text{KRR}_\lambda(\beta; \mathbb{Q}))^2 + C \cdot \frac{1 + \lambda^2}{\lambda^2} \cdot \|\beta_S\|_1, \tag{23}
\]

where \( c_j = m_\mu \cdot E \|X_j - X_j^0\|/(\|h(0)M_X^2\|) > 0 \), and \( C > 0 \) depends only on \( \mu, M_X, M_Y \).

**Remark.** According to Eq. (22), the term \( F^\text{KRR}_\lambda(0; \mathbb{Q}) - F^\text{KRR}_\lambda(\beta; \mathbb{Q}) \) on the right-hand side of Eq. (23) is approximately (when \( \lambda \) is small) equal to the difference between the total variance of \( Y \) and the unexplained variance of \( Y \) given \( X_{\text{supp}(\beta)} \), which is simply the explained variance of \( X \) given \( X_{\text{supp}(\beta)} \). Theorem 3 shows that the gradient with respect to the noise variables is lower bounded by the difference between the explanatory power of the selected variables, \( F^\text{KRR}_\lambda(0; \mathbb{Q}) - F^\text{KRR}_\lambda(\beta; \mathbb{Q}) \), and the size of the noise variables \( \|\beta_S\|_1 \).

Theorem 3 immediately implies that the kernel ridge regression objective is self-penalizing.

**Corollary 4.2.** Given Assumptions 1 and 2, and assuming \( S \not= \emptyset \), define for \( c, \delta, \lambda > 0 \) the following set:

\[
B_{c, \delta, \lambda} = \{ \beta \in X : F^\text{KRR}_\lambda(0; \mathbb{Q}) - F^\text{KRR}_\lambda(\beta; \mathbb{Q}) > c, \|\beta_S\|_1 < \delta c^2 \lambda^3 \}.
\]

The set \( B_{c, \delta, \lambda} \not= \emptyset \) whenever \( c \leq c_0, \lambda \leq \lambda_0 \). Furthermore, there exists \( \delta_0 \) such that the objective \( F^\text{KRR}_\lambda(\beta; \mathbb{Q}) \) is self-penalizing with respect to \( B_{c, \delta, \lambda} \) when \( \delta \leq \delta_0, \lambda \leq 1 \) and \( B_{c, \delta, \lambda} \not= \emptyset \).

**Proof.** We show that \( B_{c, \delta, \lambda} \not= \emptyset \) for small enough \( c, \lambda \). First, note \( F^\text{KRR}_\lambda(0; \mathbb{Q}) = \frac{1}{2} \text{Var}_Q [Y] \). Next, fix any \( \beta_0 \in \mathcal{B} \) such that \( \text{supp}(\beta_0) = S \not= \emptyset \). Using Eq. (22) yields

\[
\lim_{\lambda \to 0} F^\text{KRR}_\lambda(\beta_0; \mathbb{Q}) = \frac{1}{2} \cdot E \text{Var}[Y|X_S] < \frac{1}{2} \cdot \text{Var}_Q(Y) = F^\text{KRR}_\lambda(0; \mathbb{Q}).
\]

Hence, there exists \( c_0 > 0 \) such that \( F^\text{KRR}_\lambda(\beta_0; \mathbb{Q}) < F^\text{KRR}_\lambda(0; \mathbb{Q}) - c_0 \) for all \( \lambda \leq \lambda_0 \). As a result, \( \beta_0 \in B_{c, \delta, \lambda} \) whenever \( \lambda \leq \lambda_0, c \leq c_0 \). This proves the first part of the corollary. The rest of the corollary follows from the gradient lower bound (23) in Theorem 3. \[ \square \]

### 4.5 Proof of Theorem 2

Recalling the integral representation of the kernel function, \( h \), in Eq. (11), we have:

\[
h(z) = \int_0^\infty e^{-tz} \mu(dt) \Rightarrow h'(z) = - \int_0^\infty te^{-tz} \mu(dt), \tag{24}
\]

for some measure \( \mu \) on \( \mathbb{R}_+ \). A key observation from Eq. (24) is that both the function \( h \) and its derivative \( h' \) are mixtures of exponential functions. We shall exploit this fact to see how the gradient of the metric learning objective can be bounded by the objective itself.
Using the integral representation in Eq. (24), we have:

\[
F_{\text{ML}}(\beta; Q) = -E_Q[YY'h(\|X - X'\|_{q,\beta})] \quad \text{(25)}
\]

Similarly, we have the following representation for the gradient:

\[
\partial_{\beta_j} F_{\text{ML}}(\beta; Q) = -E_Q[YY'h'(\|X - X'\|_{q,\beta})|X_j - X'_j|^q].
\]

\[
= \int_0^\infty E_Q[YY'te^{-t\|X - X'\|_{q,\beta}}|X_j - X'_j|^q] \mu(dt).
\quad \text{(26)}
\]

Based on these representations, it remains to prove the following integral inequality from which we derive the desired relationship between $F_{\text{ML}}$ and its gradient: for any $j \in S^c$,

\[
\int_0^\infty E_Q[YY'te^{-t\|X - X'\|_{q,\beta}}|X_j - X'_j|^q] \mu(dt) \geq c(\beta) \cdot \int_0^\infty E_Q[YY'te^{-t\|X - X'\|_{q,\beta}}] \mu(dt).
\quad \text{(27)}
\]

The proof of inequality (27) is straightforward. Recalling that $E[Y|X] = f^*(X_S)$ and $X_S \perp X_{S^c}$, and using the following multiplicative property of the exponential function:

\[
e^{-\|X - X'\|_{q,\beta}} = e^{-\|X_S - X'_S\|_{q,\beta}} \cdot e^{-\|X_{S^c} - X'_{S^c}\|_{q,\beta}},
\]

we can decompose the integrand on the left-hand side of Eq. (27) into two terms:

\[
E_Q[YY'te^{-t\|X - X'\|_{q,\beta}}|X_j - X'_j|^q] = E_Q[YY'te^{-t\|X_S - X'_S\|_{q,\beta}}] \cdot E_Q[e^{-t\|X_{S^c} - X'_{S^c}\|_{q,\beta}}|X_j - X'_j|^q].
\quad \text{(28)}
\]

Now we lower bound the first term on the right-hand side:

\[
E_Q[YY'te^{-t\|X_S - X'_S\|_{q,\beta}}] \geq E_Q[YY'te^{-t\|X_S - X'_S\|_{q,\beta}}] \cdot E_Q[e^{-t\|X_{S^c} - X'_{S^c}\|_{q,\beta}}]
\]

\[
= E_Q[YY'te^{-t\|X - X'\|_{q,\beta}}].
\quad \text{(29)}
\]

Note that we have used the fact that $(x, x') \mapsto \exp(-\|x - x'\|_{q})$ is a positive definite kernel in the derivation of the inequality in Eq. (29); this guarantees that the quantities on both sides are nonnegative. Combining Eq. (29) and the decomposition (28), we derive the following lower bound for the left-hand side of Eq. (27):

\[
\int_0^\infty E_Q[YY'te^{-t\|X - X'\|_{q,\beta}}|X_j - X'_j|^q] \mu(dt) \geq \int_0^\infty E_Q[YY'te^{-t\|X_S - X'_S\|_{q,\beta}}] \cdot E_Q[e^{-t\|X_{S^c} - X'_{S^c}\|_{q,\beta}}|X_j - X'_j|^q] \mu(dt).
\quad \text{(30)}
\]
Finally, we use the assumption that \( \text{supp}(\mu) \subseteq [m_\mu, M_\mu] \), where \( 0 < m_\mu < M_\mu < \infty \), to lower bound the second term in the integral. Indeed, for all \( t \in \text{supp}(\beta) \), it is lower bounded by \( \xi(\beta) \), a quantity independent of \( t \):

\[
\mathbb{E}_Q \left[ t e^{-t\|X_\cdot \beta e - X'_{\cdot \beta e}\|_q^q |X_j - X'_{j}|^q} \right] \\
\geq m_\mu \mathbb{E}_Q \left[ e^{-M_\mu \|X_\cdot \beta e - X'_{\cdot \beta e}\|_q^q |X_j - X'_{j}|^q} \right] = \xi(\beta).
\]

(31)

Substituting Eq. (31) into Eq. (30), we obtain the target inequality (27) as desired.

**Remark**  We summarize the key elements used in the derivations:

- Completely monotone functions \( h \) and \( h' \) are mixtures of exponential functions \( \exp(-z) \).
- The derivative of the exponential function \( z \mapsto \exp(-z) \) is the negative exponential function. This supplies the foundation that allows the gradient to be bounded by the objective value.
- The exponential function is multiplicative: \( \exp(-(z_1 + z_2)) = \exp(-z_1) \cdot \exp(-z_2) \), and therefore the contributions of signal and noise variables (which are assumed independent) to the gradient can be seamlessly decomposed—any random quantities \( Z_1 \perp Z_2 \) satisfy \( \mathbb{E}[\exp(-(Z_1 + Z_2))] = \mathbb{E}[\exp(-Z_1)] \cdot \mathbb{E}[\exp(-Z_2)] \).
- The exponential function is a kernel: the mapping \( (x, x') \mapsto \exp(-\|x - x'||_q) \) is positive definite. This guarantees that all bounds are meaningful in the right direction.

The proof sheds light on the crucial need for using *nonlinear* kernels in order to obtain the self-penalization property. As we saw in Section 4.2, the objective function with the *linear* kernel is not self-penalizing.

### 4.6 Sketch of the proof of Theorem 3

The proof is based on the following representation of the gradient (see Ruan et al., 2021, Proposition 4). For any \( j \in [p] \), we have:

\[
\partial_{\beta_j} F_{\lambda}^{\text{KRR}}(\beta; Q) = -\frac{1}{\lambda} \cdot \mathbb{E}_Q[z_{\beta; \lambda}(X; Y)z_{\beta; \lambda}(X'; Y')h'(|X - X'||_q)X_j - X'_{j}|^q],
\]

(32)

where \( z_{\beta; \lambda}(x; y) = y - f_{\beta; \lambda}(\beta^{1/q} \odot x) \) denotes the residual function. Given this result, and noting the resemblance between the gradient representations of the KRR objective in Eq. (32) and that of the metric learning objective in Eq. (26), it is straightforward to translate the proof for the metric learning objective in Theorem 2 to the KRR objective. We provide the detailed proof in Appendix C.1.
The Structure of the Gradient Dynamics

We turn to a characterization of the path of projected gradient descent when applied to the metric learning and the kernel ridge regression objectives. We show that, with high probability, the gradient dynamics satisfy the following pattern (outlined in Section 3.1):

- With appropriate initialization, the gradient dynamics will enter a set \( B \subseteq \mathcal{B} \) at some finite time \( t_0 < \infty \). The set \( B \) satisfies two properties: (i) \( B \) is invariant with respect to the gradient dynamics, and (ii) the objective is self-penalizing on \( B \).

As a consequence, gradient dynamics will stay in the set \( B \) after time \( t_0 \) and force the coordinates of \( \beta \) corresponding to noise variables to 0. Section 5.1 and Section 5.2 present the analysis of the metric learning and the kernel ridge regression objectives respectively. The analysis starts with the population objective and then extends the results to finite samples.

5.1 Metric learning

We start by characterizing the dynamics of the population metric learning objective:

\[
\dot{\beta}(t) \in -\nabla F_{\text{ML}}(\beta(t); Q) - N_B(\beta(t)) \quad \text{and} \quad \beta(0) \in \mathcal{B},
\]

where \( \mathcal{B} = \{ \beta : \beta \geq 0, \|\beta\|_{\infty} \leq M\} \). Let us denote

\[
B_c = \{ \beta \in \mathcal{B} : F_{\text{ML}}(\beta; Q) < -c \}.
\]

Proposition 4. Given Assumptions 1 and 2, let \( S \neq \emptyset \) and assume \( S \subseteq \text{supp}(\beta(0)) \). Then there exists a constant \( c > 0 \) such that the trajectories \( t \mapsto \beta(t) \) satisfy the following properties:

(a) The gradient dynamics enters \( B_c \) in finite time. In fact, \( \beta(0) \in B_{3c} \subseteq B_c \).

(b) The objective \( F_{\text{ML}}(\cdot; Q) \) is self-penalizing on the set \( B_c \).

(c) The set \( B_c \) is invariant with respect to the gradient dynamics of \( F_{\text{ML}}(\cdot; Q) \).

As a consequence, there exists \( \tau < \infty \) so that \( \emptyset \nsubseteq \text{supp}(\beta(t)) \subseteq S \) for all \( t \geq \tau \).

Proof Let \( c = |F_{\text{ML}}(\beta(0); Q)|/4 > 0 \). Note \( c > 0 \) since \( \emptyset \nsubseteq S \subseteq \text{supp}(\beta(0)) \) and \( F_{\text{ML}} \) is a nonparametric dependence measure. The claim (a) is true by construction since \( \beta(0) \in B_{3c} \subseteq B_c \). Claim (b) is a restatement of the self-penalizing property (Corollary 4.1). Finally, claim (c) follows from the monotonicity of the gradient dynamics (Theorem 4). 

Next, we consider the finite-sample dynamics of the metric learning objective:

\[
\dot{\beta}(t) \in -\nabla F_{\text{ML}}(\beta(t); Q_n) - N_B(\beta(t)) \quad \text{and} \quad \beta(0) \in \mathcal{B}.
\]

We use the notation \( \tilde{\beta}(t) \) to denote the solution that is output by the finite-sample dynamics. Introduce

\[
\tilde{B}_{c,n} = \{ \beta \in \mathcal{B} : F_{\text{ML}}(\beta; Q_n) < -c \}.
\]
The definition of $\tilde{B}_{c,n}$ parallels that of $B_c$ (see Eq. (34)).

Let us define $\Omega_n(\epsilon)$ as the event on which the empirical gradients and objective values are uniformly close to their population counterparts over the feasible set $B$:

$$
|F_{\text{ML}}(\beta; Q_n) - F_{\text{ML}}(\beta; \bar{Q})| \leq \epsilon, \\
\|\nabla F_{\text{ML}}(\beta; Q_n) - \nabla F_{\text{ML}}(\beta; \bar{Q})\|_{\infty} \leq \epsilon \quad \text{for all } \beta \in B.
$$

Lemma 5.1 shows that the event $\Omega_n(\epsilon)$ occurs with high probability. The proof, which is based on standard concentration inequalities, is deferred to Section D.1.

**Lemma 5.1.** Given Assumptions 1 and 2, there exists a constant $c' > 0$ independent of $n$ such that $\Omega_n(\epsilon)$ happens with probability at least $1 - \exp(-c' n \epsilon^2)$.

Now we are ready to state the empirical analogue of Proposition 4.

**Proposition 6’.** Given Assumptions 1 and 2, and let $S \neq \emptyset$ and $S \subseteq \text{supp}(\tilde{\beta}(0))$. There exist constants $\epsilon, c, \tilde{c} > 0$ independent of $n$ such that on the event $\Omega_n(\epsilon)$, the empirical gradient dynamics $t \mapsto \tilde{\beta}(t)$ and the set $\tilde{B}_{c,n}$ satisfy the following properties:

(a) The gradient dynamics enters $\tilde{B}_{\tilde{c},n}$ in finite time.

(b) The objective $F_{\text{ML}}(\cdot; Q_n)$ is self-penalizing on the set $\tilde{B}_{\tilde{c},n}$.

(c) The set $\tilde{B}_{c,n}$ is invariant with respect to the gradient dynamics of $F_{\text{ML}}(\cdot; Q_n)$.

Hence, on the event $\Omega_n(\epsilon)$, there exists $\tau < \infty$ so that $\emptyset \subseteq \text{supp}(\beta(t)) \subseteq S$ for all $t \geq \tau$. The constant $\tau > 0$ is independent of $n$.

**Proof** Proposition 6’ is almost an immediate consequence of Proposition 4. Let $c > 0$ be a constant such that Proposition 4 holds. The following fact is used throughout the proof, which follows from the triangle inequality and the definition of $\Omega_n(\epsilon)$ for $\epsilon < c$:

$$
B_{3c} \subseteq \tilde{B}_{2c,n} \subseteq B_c \quad \text{on the event } \Omega_n(\epsilon).
$$

Set $\tilde{c} = 2c$, and note that $\tilde{\beta}(0) = \beta(0) \in B_{3c}$ by definition of $c$ (see Proposition 4). Hence $\tilde{\beta}(0) \in \tilde{B}_{c,n}$ on the event $\Omega_n(\epsilon)$ by virtue of Eq. (38).

Next, we show that for some $0 < \epsilon \leq c$, the objective $F_{\text{ML}}(\cdot; Q_n)$ is self-penalizing on $\tilde{B}_{c,n}$ on the event $\Omega_n(\epsilon)$. Proposition 4 says that $F_{\text{ML}}(\beta; Q)$ is self-penalizing on the set $B_c$. Hence the population gradient $\partial_{\beta} F_{\text{ML}}(\beta; Q)$ has a uniform lower bound $\epsilon > 0$ over the set of $\beta \in B_c$ for noise variables $j \notin S$. Let us pick $\epsilon = c/2 \wedge c$. On the event $\Omega_n(\epsilon)$, the empirical gradient $\partial_{\beta} F_{\text{ML}}(\beta; Q_n)$ has a uniform lower bound $\epsilon/2 > 0$ over $\beta \in B_c$ and $j \notin S$ (by the triangle inequality). This implies $B_{\tilde{c},n} \subseteq B_c$ on $\Omega_n(\epsilon)$.

Finally, the invariance of $\tilde{B}_{c,n}$ follows from the monotonicity of the gradient dynamics (Theorem 4). □

**Proof of Theorem 1A** Theorem 1A follows from Proposition 6’ and Lemma 5.1.
5.2 Kernel ridge regression

In this section we characterize the gradient dynamics of the population kernel ridge regression (KRR) objective:

$$\dot{\beta}(t) \in -\nabla F^K_{\lambda}(\beta(t); Q) - N_B(\beta(t)) \quad \text{and} \quad \beta(0) \in \mathcal{B},$$

(39)

where $\mathcal{B} = \{\beta \in \mathbb{R}^p : \|\beta\|_\infty \leq M\}$. Let us denote

$$B_{c,\delta,\lambda} = \{\beta \in \mathcal{B} : F^K_{\lambda}(\beta; Q) - F^K_{\lambda}(0; Q) < -c, \|\beta_S\|_1 < c^2 \delta \lambda^3\}. \quad (40)$$

Let $\hat{S} = \{l \in \mathcal{S} : \text{Var}_Q(\mathbb{E}_Q[Y|X_l]) \neq 0\}$ denote the set of main effects.

**Proposition 7.** Given Assumptions 1 and 2, assume $\hat{S} \neq \emptyset$. Set $q = 1$ and $\beta(0) = 0$. There exist constants $c, C, \delta, \lambda_0 > 0$ such that the following holds for any $\lambda \leq \lambda_0$:

(a) The gradient dynamics enters $B_{3c,\delta/81,\lambda} \subseteq B_{c,\delta,\lambda}$ at the time $t = C\lambda^2$.

(b) The objective $F^K_{\lambda}(\cdot; Q)$ is self-penalizing on the set $B_{c,\delta,\lambda}$.

(c) The set $B_{c,\delta,\lambda}$ is invariant with respect to the gradient dynamics of $F^K_{\lambda}(\cdot; Q)$.

As a consequence, there exists $\tau < \infty$ so that $\emptyset \subset \text{supp}(\beta(t)) \subseteq \mathcal{S}$ for all $t \geq \tau$.

**Proof** We sketch the proof of Proposition 7; for a detailed proof, see Appendix C.6.

To prove (a), note that to enter $B_{3c,\delta/81,\lambda}$ by time $t = C\lambda^2$, the gradient dynamics must (i) decrease the objective value sufficiently quickly (shown by Lemma 5.2 below), and (ii) keep $\|\beta_S(t)\|_1$ small. For (ii), note that $\|\beta_S(0)\|_1 = 0$ for all $t > 0$ since the self-penalizing property (Theorem 4) implies $\partial_{\beta_j} F^K_{\lambda}(\beta; Q) \geq 0$ for all $j \notin \hat{S}$ when $\text{supp}(\beta) \subseteq \mathcal{S}$.

Claim (b) is simply a restatement of the self-penalizing property (see Corollary 4.2).

For claim (c), note that the self-penalizing property (Corollary 4.2) guarantees that $\|\beta_{S^c}\|_1$ will always be decreasing on $B_{c,\delta,\lambda}$. This fact combined with the monotonicity of the gradient dynamics (Theorem 4) implies the claim.

**Lemma 5.2.** Given Assumptions 1 and 2, and assuming $\hat{S} \neq \emptyset$, set $q = 1$ and $\beta(0) = 0$. There exist constants $\lambda_0, c, C > 0$ such that the following holds for any $\lambda \leq \lambda_0$:

$$F^K_{\lambda}(\beta(t); Q) \leq F^K_{\lambda}(\beta(0); Q) - c \quad \text{when} \quad t \geq C\lambda^2.$$  

(41)

**Proof** The result is a consequence of two results: (i) the Lyapunov convergence theorem for gradient inclusion, which says that the objective value has a certain rate of decay governed by the size of the gradient along the trajectory:

$$F^K_{\lambda}(\beta(t); Q) \leq F^K_{\lambda}(\beta(0); Q) - \int_0^t \|g^*(\beta(s))\|_2^2 ds,$$

(42)

where the mapping $g^*(\beta) := \text{argmin}\{\|g\|_2 : g \in \nabla F^K_{\lambda}(\beta; Q) + N_B(\beta)\}$ is the minimum norm gradient at $\beta$, and (ii) a lower bound on the size of the kernel ridge regression gradient.
at the beginning stage of the differential inclusion. The details of the proof of Lemma 5.2 are given in Section C.5.

Next, we consider the finite-sample dynamics of the kernel ridge regression objective: \[
\dot{\beta}(t) \in -\nabla F^\text{KRR}_\lambda(\beta(t); Q_n) - N_B(\beta(t)) \quad \text{and} \quad \beta(0) \in B.
\]

Let \(\tilde{\beta}(t)\) denote the solution of the finite-sample dynamics. Introduce \(\tilde{B}_{c,\delta,\lambda,n} = \{ \beta \in B : F^\text{KRR}_\lambda(\beta; Q_n) - F^\text{KRR}_\lambda(0; Q_n) < -c, \|\beta_S\|_1 < c^2\delta\lambda^3 \}\).

The definition of \(\tilde{B}_{c,\delta,\lambda,n}\) parallels that of \(B_{c,\delta,\lambda}\) (see Eq. (40)). Introduce \(\Omega_n(\epsilon)\), defined as the event on which the empirical and population gradients and objective values are uniformly close over the feasible set \(B\):

\[
\left| F^\text{KRR}_\lambda(\beta; Q_n) - F^\text{KRR}_\lambda(\beta; Q) \right| \leq \epsilon,
\|
\nabla F^\text{KRR}_\lambda(\beta; Q_n) - \nabla F^\text{KRR}_\lambda(\beta; Q) \nabla F^\text{KRR}_\lambda(\beta; Q) \|_\infty \leq \epsilon
\]

(45)

Lemma 5.3 shows that the event \(\Omega_n(\epsilon)\) happens with high probability. The proof, which is based on standard concentration inequalities, is deferred to Appendix D.2.

**Lemma 5.3.** Given Assumptions 1 and 2, assume \(\lambda \leq 1\). Then the event \(\Omega_n(\epsilon)\) happens with probability at least \(1 - \exp(-c' n\epsilon^2\lambda^6)\) for any \(\epsilon > 0\). Here \(c'\) is independent of \(n, \lambda\).

Recall that \(\hat{S} = \{ l \in S : \text{Var}_Q(\mathbb{E}_Q[Y|X_l]) \neq 0 \}\) denotes the set of main effects.

**Proposition 7'.** Given Assumptions 1 and 2, assume \(\hat{S} \neq \emptyset\), and set \(q = 1\) and \(\tilde{\beta}(0) = 0\). Let \(\lambda \leq 1\). There exist constants \(\bar{c}, \bar{C}, \bar{c}_1, \bar{c}_2, \bar{c}_3 > 0\) independent of \(n\) such that for any \(\lambda \leq \lambda_0\) the empirical gradient dynamics \(t \mapsto \beta(t)\) satisfies the following on the event \(\Omega_n(\epsilon\lambda)\):

(a) The gradient dynamics enters \(\tilde{B}_{c,\delta,\lambda,n}\) at the time \(t = \bar{C}\lambda^2\).

(b) The objective \(F^\text{KRR}_\lambda(\cdot; Q)\) is self-penalizing on the set \(\tilde{B}_{c,\delta,\lambda,n}\).

(c) The set \(\tilde{B}_{c,\delta,\lambda,n}\) is invariant with respect to the gradient dynamics of \(F^\text{KRR}_\lambda(\cdot; Q)\).

As a consequence, there exists \(\tau < \infty\) so that \(\emptyset \subset \supp(\beta(t)) \subset S\) for all \(t \geq \tau\) on the event \(\Omega_n(\epsilon\lambda)\). Furthermore, we can choose \(\tau\) to be \(\tau = \bar{c}\lambda^2\) where \(\bar{c}\) is independent of \(\lambda, n\).

**Proof** Proposition 7' follows from its population version (Proposition 7), and a Grönwall deviation bound that controls the difference between the population and empirical trajectories (see Lemma C.1). For details, see Section C.7.

**Proof of Theorem 1B** Theorem 1B follows from Proposition 7' and Lemma 5.3
6 Statistical Implications

This section shows how we can leverage self-penalizing objectives to develop procedures that consistently select signal variables without any need for $\ell_1$ regularization. In Section 5, we showed that, when properly initialized, gradient flow applied to a self-penalizing objective converges to a stationary point which automatically excludes all noise variables. That is, $\hat{S} \subseteq S$, where $\hat{S} = \text{supp}(\hat{\beta})$ is the support of the stationary point found by gradient flow. Note, however, that we do not have the guarantee that $\mathbb{E}[Y|X] = \mathbb{E}[Y|X_{\hat{S}}]$; i.e., we may miss relevant variables. Indeed, counterexamples show that relevant variables can be missing from even the global minima of the population objective (Liu and Ruan, 2020).

Below we show how to use the metric learning and kernel ridge regression objectives to construct $\hat{S}$ such that (i) $\hat{S} \subseteq S$ and (ii) $\mathbb{E}[Y|X] = \mathbb{E}[Y|X_{\hat{S}}]$. There is enough similarity in the algorithms used for these two objectives to abstract out a recipe. Adaptation of this recipe may be useful when designing selection algorithms based on other self-penalizing objectives, although no general theory is pursued here. The recipe involves solving a sequence of minimization problems. At each iteration $k$ in the sequence, the minimizing problem we solve depends on the variables that have been selected prior to iteration $k$, denoted $\hat{S}(k)$. The objective function $F(\beta; Q_{\hat{S}(k)})$, the constraint set $B_{\hat{S}(k)}$ and the initializer, $\beta(0; \hat{S}(k))$, can all depend on $\hat{S}(k)$.

Our recipe proceeds as follows:

1. Initialize $\hat{S}(0) = \emptyset$ and $k = 0$.
2. Run gradient descent to minimize $F(\beta; Q_{\hat{S}(k)})$ over the constraint set $B_{\hat{S}(k)}$ starting from initialization $\beta(0; \hat{S}(k))$. Let $\hat{\beta}(k)$ be the solution.
3. Update $\hat{S}(k+1) = \hat{S}(k) \cup \text{supp}(\hat{\beta}(k))$.
4. Perform a statistical test for the null hypothesis $H_0 : \mathbb{E}[Y|X_{\hat{S}(k+1)}] = \mathbb{E}[Y|X_{\hat{S}(k)}]$. If rejected, return to Step 2 and increment $k = k + 1$. Else, return $\hat{S} = \hat{S}(k)$.

Intuitively, the minimization problem in Step 2 should be set up with the goal of finding a set of variables that is predictive of $Y$ conditional on the selected variables in $S(k)$. The specifics of how to do this will vary with the type of self-penalizing objective since it depends on the mechanism by which an objective tries to detect signal. Section 6.1 describes the sequence of minimization problems used for the metric learning objective and Section 6.2 for the kernel ridge regression objective.

Remark It is natural to wonder why Step 4 is even necessary if a self-penalizing objective automatically controls false positives. A careful review of Theorems 1A and 1B shows that a necessary condition for the metric learning and kernel ridge regression objectives to be self-penalizing is that $S \neq \emptyset$. Therefore, the step is needed in the first iteration, $k = 1$, to ensure that the signal set $S$ is not empty. Additionally, once all the relevant variables have been included in $\hat{S}(k)$, the objective in the subsequent iteration of Step 2 may no longer be self-penalizing (see Section 6.1); hence the need for Step 4.

\[\text{The precise meaning of the notation } \mathbb{E}[Y|X_{\hat{S}}] \text{ is as follows. We take a sample } (X, Y) \text{ (a test sample) independent from the raw data and evaluate its conditional expectation } \mathbb{E}[Y|X_{\hat{S}}].\]
Remark Why use a self-penalizing objective to select variables if in the end we must apply a nonparametric test to ascertain the validity of the discovered variables? One can certainly build variable selection procedures using only nonparametric conditional independence tests (Fukumizu et al., 2007; Vergara and Estévez, 2014; Azadkia and Chatterjee, 2019) but such procedures would either require conducting exponentially many tests (over subsets of variables) or would require additional assumptions about the signal, e.g., that the signal is hierarchical. In contrast, our procedure computes at most \( p \) conditional independence tests and possesses statistical guarantees even for non-hierarchical signals; see, e.g., Proposition 8. The procedure attains these attractive properties by using a self-penalizing objective to generate a sequence of candidate variable sets to which we apply a nonparametric conditional test.

6.1 Classification: Metric learning algorithm

The metric learning algorithm, Algorithm 1, uses the metric learning objective to consistently select signal variables in a classification setting. Proposition 8 shows that the variables selected by Algorithm 1 achieves (i) \( \hat{S} \subseteq S \) and (ii) \( \mathbb{E}[Y|X] = \mathbb{E}[Y|X_{\hat{S}}] \). In Algorithm 1 we solve a sequence of minimization problems where the minimizing objective at each step depends on the currently selected variables, \( \hat{S} \). Let \( Q \) and \( Q_n \) denotes the population and empirical distribution of the data. For any subset of features, \( X_A \), we define the reweighted distribution \( Q_{\hat{S}}^n \) as follows:

\[
\frac{dQ_{\hat{S}}^n}{dQ_n}(x, y) \propto Q(Y = -y|X_A = x_A).
\] (46)

The minimization objective used in each step is the metric learning objective with respect to the weighted distribution \( Q_{\hat{S}}^n \). The reweighting has the effect of removing the effect of the selected variables, \( X_{\hat{S}} \), while leaving intact any signal attributable to the unselected variables. See Liu and Ruan (2020) for further details.

Remark To evaluate \( Q_{\hat{S}}^n \) in practice, we need a nonparametric estimate of the population conditional distribution \( Q(Y|X_{\hat{S}}) \) (see equation (46)). In our proof of Proposition 8, we will ignore this estimation error and simply pretend that \( Q(Y|X_{\hat{S}}) \) is available. With some work, one can adapt our results to the case of estimated \( Q(Y|X_{\hat{S}}) \). Primarily, the threshold \( \epsilon_n \) must be increased to account for the additional noise in the estimation process.

Proposition 8. Given Assumptions 1 and 2, assume \( \mathbb{E}_Q[\text{Var}_Q(Y|X)] > 0 \). Fix an initialization \( \beta^{(0)} \) that satisfies \( \text{supp}(\beta^{(0)}) = [p] \). There exist constants \( C, c, \epsilon_0 > 0 \) independent of \( n \) such that the following holds. With probability at least \( 1 - 2^{|S|} e^{-cn^2} \), for the choice of the threshold \( \epsilon_n \geq C/\sqrt{n} \), the output \( \hat{S} \) of Algorithm 1 satisfies (i) \( \hat{S} \subseteq S \), and (ii) \( \mathbb{E}[Y|X] = \mathbb{E}[Y|X_{\hat{S}}] \) if \( \epsilon_n \leq \epsilon_0 \) in addition.

6.2 Regression: Kernel Ridge Regression Algorithm

Algorithm 2 selects variables by repeatedly minimizing the KRR objective. While the same KRR objective is used in each minimization problem, the initialization and feasible region
Algorithm 1 Empirical Metric Learning Procedure

Require: Initializer $\beta^{(0)}$, $M > 0$ and $\epsilon_n > 0$
Ensure: Initialize $\hat{S} = \emptyset$.
1: while $\hat{S}$ not converged do
2: Run projected gradient descent (with initialization $\beta^{(0)}$) to solve
   \[
   \min_{\beta} F_{\lambda_n}^{\text{ML}}(\beta; Q_n) \quad \text{subject to} \quad \beta \geq 0, \quad \|\beta\|_\infty \leq M.
   \]
3: Update $\hat{S} = \hat{S} \cup \operatorname{supp}(\hat{\beta})$ if $F_{\lambda_n}^{\text{ML}}(\beta; Q_n) < -\epsilon_n$.
4: end while

Differ depending on what variables have been selected so far. Suppose $\hat{S}$ has already been selected. For the next minimization problem:

- Initialize at $\beta(0; \hat{S})$ where $\beta_{S,0}(0; \hat{S}) = 0$ and $\beta_{\hat{S},0}(0; \hat{S}) = M1_{\hat{S}}$.
- Restrict the minimization to the feasible set $B_{\hat{S}} = \{\|\beta\|_\infty \leq M \quad \text{and} \quad \beta_{\hat{S}} = M1_{\hat{S}}\}$.

That is, the variables selected in prior rounds of minimization will always be kept active in subsequent rounds. This choice of initialization and constraint region ensures that we do not miss possible interaction signals between selected and unselected variables. Proposition 9 shows that Algorithm 2 achieves (i) $\hat{S} \subseteq S$ and (ii) $E[Y|X] = E[Y|X_{\hat{S}}]$ upon termination.

Algorithm 2 Empirical Kernel Ridge Regression Procedure

Require: Initializer $\beta(0; \emptyset)$, $M > 0$ and $\epsilon_n > 0$.
1: while $\hat{S}$ not converged do
2: Run projected gradient descent (with initialization $\beta(0; \hat{S})$) to solve
   \[
   \min_{\beta} F_{\lambda_n}^{\text{KRR}}(\beta; Q_n) \quad \text{subject to} \quad \beta \geq 0, \quad \|\beta\|_\infty \leq M \quad \text{and} \quad \beta_{\hat{S}} = M1_{\hat{S}}.
   \]
3: Update $\hat{S} = \hat{S} \cup \operatorname{supp}(\hat{\beta})$ if $F_{\lambda_n}^{\text{KRR}}(\beta; Q_n) > \epsilon_n$, where $\beta_{\hat{S}}$ is defined by $\beta_{\hat{S}} = M1_{\hat{S}}$ and $\beta_{\hat{S}} = 0$.
4: end while

Due to the nature of the provable self-penalizing mechanism for the KRR objective (Theorem 1B), we require the following hierarchical signal assumption.

Assumption 3 (Hierarchical signal). For any subset $T \subseteq S$ for which $E[Y|X] \neq E[Y|X_T]$, there exists an index $j \in S \setminus T$ such that $E[Y|X_T] \neq E[Y|X_T \cup (j)]$.

Proposition 9. Given Assumptions 1-3, let the initializers $\{\beta(0; T)\}_{T \subseteq [p]}$ be as follows: $
\beta(0; T) = M1_T \quad \text{and} \quad \beta(0; T)_{T} = 0$. Set $q = 1$. There exist constants $c, C, \lambda_0, \epsilon_0 > 0$ independent of $n$ such that the following holds. For any parameter $\lambda_n \leq \lambda_0$ and threshold $\epsilon_n \geq C/(\sqrt{n}A_n^2)$, we have that with probability at least $1 - e^{-c_n\lambda_n^2(\epsilon_n^2+A_n^2)}$, the output of Algorithm 2 satisfies (i) $\hat{S} \subseteq S$ and (ii) $E[Y|X] = E[Y|X_{\hat{S}}]$ if $\epsilon_n \leq \epsilon_0$ in addition.
7 Experiments

Our theory has established the existence of the self-penalization phenomenon—that the finite-sample solutions of kernel-based optimization are naturally sparse—under the following conditions:

- Exact independence or weak dependence between the signal and the noise variables.
- Existence of certain type of signal variables (e.g., the main effect signal for the KRR).

In this section we present the results of numerical experiments that corroborate the theory. These experiments also suggest that the self-penalization phenomenon occurs in a broader range of settings than what are currently able to establish theoretically.

7.1 The effect of correlation

Our first set of experiments investigates how correlation structures between the covariates affect the self-penalization. The experimental settings are as follows. We draw the covariates \( X \) from a normal distribution whose covariance structure follows a standard autoregressive model, where \( \text{Cov}(X_i, X_j) = \rho^{|i-j|} \), for \( 1 \leq i, j \leq p \), and where a parameter \( \rho \in [-1, 1] \) that measures the strength of the correlations. The response \( Y \) is constructed as follows.

- In the classification setting, we construct the label \( Y = U \text{ sign}(f(X)) \). Here \( f(X) \) is the signal and \( U \in \{\pm 1\} \) is independent noise with \( P(U = 1) = 1 - P(U = -1) = \epsilon \).
- In the regression setting, we construct the label \( Y = f(X) + \epsilon \cdot U \). Here \( f(X) \in \mathbb{R} \) is the true signal, \( U \sim \mathcal{N}(0, 1) \) is independent noise and \( \epsilon > 0 \) is the noise level.

We set the initialization \( \beta_i^{(0)} = 1/p \) for \( i \in [p] \) and the stepsize \( \alpha = 1 \).

We begin by considering the results of two simple experiments that explore the role of correlation. In the first setup, we consider a simple situation in which there are only two covariates \( X_1, X_2 \). We define a linear signal, \( f(X) = X_1 \), so that \( X_1 \) is the only signal variable. We set \( n = 200 \) samples, \( p = 2 \) features, and noise level \( \epsilon = 0.1 \). We choose the correlation parameter \( \rho \) from the set \( \{-1, -0.9, -0.8, \ldots, +0.8, +0.9, +1\} \). For both classification and regression, we run gradient descent on the metric learning objective and kernel ridge regression for 100 steps. In this setup our finding is that the algorithm always only picks up the true variable \( X_1 \) as long as \( \rho \neq \pm 1 \). In other words, as long as the features are not perfectly correlated, the algorithm automatically penalizes the noise variable \( X_2 \) and shrinks its coefficient \( \beta_2 \) to exactly 0. Note the same behavior does not happen if we run a linear least square (without \( \ell_1 \) penalization); in that case we always obtain dense solutions (i.e., \( \beta_1 \neq 0, \beta_2 \neq 0 \)).

In the second setup, we consider the case where \( f(X) = X_1^3 + X_2^3 \) is a nonlinear signal that involves two signal variables. The setup has \( n = 300 \) samples, \( p = 10 \) features, and noise level \( \epsilon = 0.1 \). We choose the correlation parameter \( \rho \) from the set \( \{-1, -0.9, -0.8, \ldots, +0.8, +0.9, +1\} \), and we observe that with extremely high probability (\( \geq 99\% \)) the algorithms only pick up the two signal variables \( X_1, X_2 \) as long as the features are not perfectly correlated; i.e., \( \rho \neq \pm 1 \). This shows that the self-penalization can occur in the presence of strong correlations.
7.2 Kernel ridge regression always yields self-penalization

This section presents numerical evidence showing that the kernel ridge regression performs self-penalization even if the data has no main effect signals (as required in Theorem 1B).

The experimental setup is as follows. Draw the covariate \( X \) where the coordinates are i.i.d., \( X_i \sim \mathcal{N}(0, 1) \), and the response is \( Y = f(X) + \epsilon \cdot U \), where the signal \( f(X) = X_1X_2 \) and the noise \( U \sim \mathcal{N}(0, 1) \). Under this setup, although \( X_1, X_2 \) are signal variables, they are not main effect signals since \( \mathbb{E}[f(X) \mid X_1] = \mathbb{E}[f(X) \mid X_2] = 0 \) (we call such signal variables “pure interaction signals”). In the experiments, we set \( n = 200, p = 10, \) and \( \epsilon = 0.1 \). We set the ridge penalty \( \lambda = 0.01 \), the gradient descent stepsize \( \alpha = 1 \) and the initialization \( \beta(0) \) where \( \beta_i(0) = 1/p \) for \( i \in [p] \).

Our results are the following. Among all the 100 repeated experiments, the kernel ridge regression algorithm always includes all the pure interaction signal variables \( X_1, X_2 \), and excludes the noise variables \( X_3, X_4, \ldots, X_{10} \). This numerical evidence suggests the kernel ridge regression is able to self-penalize in the absence of main effects.

7.3 Performance in finite samples

Finally, we conduct further numerical experiments to illustrate the self-penalization phenomenon under different choices of the ratio \( n/p \). We consider different forms of the signal in our experiments. In all experiments, we draw the covariates \( X \) from a standard normal distribution where each coordinate is independently \( X_i \sim \mathcal{N}(0, 1) \).

Main effect  Our first setup is the main effect model.

- In the classification setting, we simulate the logistic model, \( \text{logit}(Y \mid X) = X_1 \).
- In the regression setting, we simulate \( Y = X_1 + \mathcal{N}(0, 1) \).

We fix the sample size \( n = 50 \) and choose the dimensionality \( p \) in the range from 20 to 400. Figure 3 reports the true positive and false positive rate across different choices of \( p \).

![Figure 3](image)

**Figure 3.** True positive rate and false positive rate curve under the main effect model against different choice of dimensionality \( p \). Here the sample size \( n = 50 \) is fixed.
**Pure Interaction**  Our second setup is the pure interaction model.

- In the classification setting, we simulate the logistic model, \( \logit(Y|X) = 2X_1X_2 \).
- In the regression setting, we simulate \( Y = X_1X_2 + N(0, 1) \).

We fix the sample size \( n = 200 \) and tune the dimensionality \( p \) from 10 to 50. Figure 4 reports the true positive and false positive rate across different choices of \( p \).

**Figure 4.** True positive rate and false positive rate curve under the pure interaction model against different choice of dimensionality \( p \). Here the sample size \( n = 200 \) is fixed.

### 8 Discussion

We have described a new sparsity-inducing mechanism based on minimization over a family of kernels. The mechanism does not involve classical explicit regularization (such as \( \ell_1 \) penalization, early stopping etc.), yet we find that in many cases the mechanism is able to generate solutions that are exactly sparse in finite samples. We coin this phenomenon self-penalization. We develop a theory that provides sufficient conditions under which the phenomenon arises, showing in particular that in cases where there are two complementary subsets of variables that are weakly dependent, the self-penalization is largely attributed to the self-penalizing property of the objective—a property that is exhibited by (nonlinear) kernel-based objectives.

The sparsity-inducing mechanism in our work is closely related to the notion of implicit regularization in the literature, which—broadly defined—means that the optimization algorithms are biased towards certain type of structured solutions. In particular, our results illustrate that the gradient-type algorithms (e.g., gradient descent), when applied to the properly designed kernel-based objectives, are automatically biased towards solutions that are sparse.

There are nonetheless several important distinctions between our work and existing work on the implicit regularization. In particular, most existent work on implicit regularization focuses on exploring and explaining the connection between the \( \ell_2 \) regularization and the gradient descent \[ \text{[Bühlmann and Yu 2003]} \, \text{[Friedman and Popescu 2004]} \, \text{[Yao et al. 2007]} \]
— in this case the focus is not on generation of sparse solutions. Indeed, there is a paucity of work in which implicit regularization is associated with solutions that are exactly sparse. The main exception is in the boosting literature, where it is shown that the coordinate descent tends towards sparse solutions (Friedman et al., 2001; Zhang and Yu, 2005; Telgarsky, 2013). For instance, least squares gradient boosting, which is steepest coordinate descent, generates a sparse regularization path (Friedund et al., 2017).

Our work also has a natural connection to the literature on sparse recovery (Bühlmann and van De Geer, 2011; Hastie et al., 2019); indeed, it can be viewed as introducing a new sparsity-inducing mechanism that can be employed to aid in the design of algorithms that are consistent in recovery of features.

Finally, we note some natural extensions of the results in the paper that are worthy of further exploration. First, one can consider discrete projected gradient descent in place of continuous gradient flow. Our results go through as long as the stepsize $\alpha$ satisfies $\alpha \leq 1/L$ where $L$ is the Lipschitz constant of the gradient of the kernel feature selection objective. Second, it is worth investigating various relaxations of the use of full gradient descent. These would include replacing full gradient descent by other deterministic gradient-type methods such as coordinate descent or accelerated gradient descent, as well as stochastic methods.

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A Preliminaries on Kernel Ridge Regression

This section presents some basic properties of kernel ridge regression (KRR). Several of our technical results are drawn from [Ruan et al. 2021] and we refer the reader to that paper for further exposition.

We consider the following family of kernel ridge regression problems. Fix a given Hilbert space $\mathcal{H}$ whose kernel is given by $k(x, x') = h(\|x - x'\|_q^q)$ where $h \in C^\infty[0, \infty)$ is a completely monotone function and $q \in \{1, 2\}$. Consider a problem indexed by $\beta \in \mathbb{R}^p_+$

$$\text{KRR}(\beta) : \minimize_{f \in \mathcal{H}} \frac{1}{2} E_Q[(Y - f(\beta^{1/q} \odot X))^2] + \frac{\lambda}{2} \|f\|_\mathcal{H}^2.$$  (47)

**Notation** Let $f_{\beta;\lambda}$ denote the minimizer of the KRR problem. Let $r_{\beta;\lambda}(x, y) = y - f_{\beta;\lambda}(x)$ and $z_{\beta;\lambda}(x, y) = y - f_{\beta;\lambda}(\beta^{1/q} \odot x)$.

### A.1 General properties ($q = 1$ or $q = 2$)

This section provides general properties of KRR when $q = 1$ or $q = 2$.

**Main Results** Our first set of results gives the characterization of the minimum $f_{\beta;\lambda}$.

**Lemma A.1** (KKT Characterization). The following identity holds for any function $g \in \mathcal{H}$:

$$E_Q\left[z_{\beta;\lambda}(X; Y)g(\beta^{1/q} \odot X)\right] = \lambda \langle f_{\beta;\lambda}, g \rangle_\mathcal{H}. \quad (48)$$

**Proof** This is Proposition 9 in [Ruan et al. 2021]. □

As a consequence of the KKT condition, we derive the following important connections between the regression function $f_{\beta;\lambda}$ and the residual function $z_{\beta;\lambda}$.

**Lemma A.2** (Balance between minimum $f_{\beta;\lambda}$ and residual $z_{\beta;\lambda}$). The following identity holds:

$$E_Q\left[z_{\beta;\lambda}(X; Y)z_{\beta;\lambda}(X'; Y')h(\|X - X'\|_q^q)\right] = \lambda^2 \|f_{\beta;\lambda}\|_\mathcal{H}^2. \quad (49)$$

**Proof** By Lemma A.1 the following identity holds for all function $g \in \mathcal{H}$:

$$E_Q\left[z_{\beta;\lambda}(X; Y)g(\beta^{1/q} \odot X)\right] = \lambda \langle f_{\beta;\lambda}, g \rangle_\mathcal{H}. \quad (50)$$

According to the reproducing property of the kernel function $k$, we can rewrite the left-hand side of Eq. (50) and obtain the following identity that holds for all function $g \in \mathcal{H}$:

$$\langle E_Q\left[z_{\beta;\lambda}(X; Y)k(\beta^{1/q} \odot X, \cdot)\right], g \rangle_\mathcal{H} = \lambda \langle f_{\beta;\lambda}, g \rangle_\mathcal{H}. \quad (51)$$

---

\[\text{Note: } r_{\beta;\lambda}(x, y) = y - f_{\beta;\lambda}(x) \text{ is the only residual function that appears in the cited paper [Ruan et al. 2021].}\]
Let \( B_H(1) \) denote the unit ball of \( H \) (i.e., \( B_H(1) = \{ g \in H : \| g \|_H \leq 1 \} \)). Now we take supremum over all possible \( g \in B_H(1) \) in the unit ball on both sides of the Eq. (51). This gives us

\[
\left\| \mathbb{E}_Q \left[ z_{\beta;\lambda}(X;Y)k(\beta^{1/q} \circ X, \cdot) \right] \right\|_H = \lambda \| f_{\beta;\lambda} \|_H.
\]

(52)

To finalize the proof of Lemma A.2, we square both sides of Eq. (52). Note then using the Cauchy-Schwartz inequality and Lemma A.3, we immediately obtain

\[
\| F_{\beta;\lambda} \|_2^2 \leq \mathbb{E}_Q [Y]^2 \cdot \mathbb{E}_Q [f_{\beta;\lambda}(\beta^{1/q} \circ X)^2] \leq |h(0)|_q \cdot \| f_{\beta;\lambda} \|_H^2.
\]

(53)

In the first step (i), we introduce independent variables \( X' \sim X \sim Q \), and in the second step (ii), we use the fact that the inner product \( \langle \cdot, \cdot \rangle_H \) is bilinear, and in the last step (iii), we use the reproducing property of the kernel function \( k \). \( \Box \)

**Lemma A.3** (Relations of Different Norms). Any function \( f \) satisfies \( \| f \|_\infty \leq |h(0)|^{1/2} \| f \|_H \).

**Proof** The evaluation functional \( F_x : f \mapsto f(x) \) is a bounded operator for all \( x \) with the operator norm uniformly bounded by \( |h(0)|^{1/2} \) (as \( H \) has the kernel \( h(\|x - x'\|_q^2) \)). \( \Box \)

**Lemma A.4** (Lower Bound of \( \| f_{\beta;\lambda} \|_H^2 \)). The following holds for all \( \beta \):

\[
\| f_{\beta;\lambda} \|_H^2 \geq \frac{1}{|h(0)| M_Y^2} (F_{\lambda}^{KRR}(0; Q) - F_{\lambda}^{KRR}(\beta; Q))^2.
\]

(54)

**Proof** Note that \( f_{0;\lambda} = 0 \) since \( \mathbb{E}_Q[Y] = 0 \) by assumption. As its consequence, we obtain

\[
F_{\lambda}^{KRR}(0; Q) = \frac{1}{2} \mathbb{E}_Q[Y^2].
\]

As a result, we obtain the following elementary upper bound on \( F_{\lambda}^{KRR}(0) - F_{\lambda}^{KRR}(\beta) \):

\[
F_{\lambda}^{KRR}(0; Q) - F_{\lambda}^{KRR}(\beta; Q) = \mathbb{E}_Q[Y f_{\beta;\lambda}(\beta^{1/q} \circ X)] - \frac{1}{2} \mathbb{E}_Q[f_{\beta;\lambda}(\beta^{1/q} \circ X)^2] - \frac{\lambda}{2} \| f_{\beta;\lambda} \|_H^2 \leq \mathbb{E}_Q[Y f_{\beta;\lambda}(\beta^{1/q} \circ X)].
\]

Using the Cauchy-Schwartz inequality and Lemma A.3, we immediately obtain

\[
(F_{\lambda}^{KRR}(0; Q) - F_{\lambda}^{KRR}(\beta; Q))^2 \leq \mathbb{E}_Q[Y]^2 \cdot \mathbb{E}_Q[f_{\beta;\lambda}(\beta^{1/q} \circ X)^2] \leq |h(0)| M_Y^2 \cdot \| f_{\beta;\lambda} \|_H^2.
\]

\( \Box \)
Lemma A.5 (Representation of $F^{KRR}_\lambda(\beta; Q)$). The following holds for all $\beta$:

$$F^{KRR}_\lambda(\beta) = \frac{1}{2} E[z_{\beta, \lambda}(X; Y) Y].$$

Proof Our starting point is the following identity. By Lemma A.1, we have

$$\lambda \|f_{\beta, \lambda}\|^2_H = E_Q \left[z_{\beta, \lambda}(X; Y) f_{\beta, \lambda}(\beta^{1/q} \circ X)\right]$$

Note $f_{\beta, \lambda}(x, y) = y - z_{\beta, \lambda}(x; y)$ by definition. As a result, we obtain the identity

$$F^{KRR}_\lambda(\beta; Q) = \frac{1}{2} E_Q [z_{\beta, \lambda}(X; Y)^2] + \frac{\lambda}{2} \|f_{\beta, \lambda}\|^2_H = \frac{1}{2} E_Q [z_{\beta, \lambda}(X; Y) Y].$$

\[ \square \]

Lemma A.6 (Representation of $\nabla F^{KRR}_\lambda(\beta; Q)$). The following holds for all $\beta$ and $l \in [p]$,

$$\partial_{\beta_l} F^{KRR}_\lambda(\beta; Q) = -\frac{1}{\lambda} E \left[z_{\beta, \lambda}(X; Y) z_{\beta, \lambda}(X', Y') h'(\|X - X'|^q_{\beta, \lambda}) |X_l - X'_l|^q\right].$$

Proof This is Proposition 4 in Ruan et al. (2021). \[ \square \]

Lemma A.7 (Lipschitzness of $\beta \mapsto \nabla F^{KRR}_\lambda(\beta; Q)$). The following bound holds for all $\beta, \beta'$:

$$\|\nabla F^{KRR}_\lambda(\beta; Q) - \nabla F^{KRR}_\lambda(\beta'; Q)\| \leq \frac{1}{\lambda^2} \cdot (2M_X)^q \cdot M_Y^2 \cdot (2|h'(0)|^2 + \lambda|h''(0)|) \cdot \|\beta - \beta'\|_1.$$ 

Proof This is Lemma C.7 in Ruan et al. (2021). \[ \square \]

Lemma A.8 (Uniform Boundedness of $\beta \mapsto \nabla F^{KRR}_\lambda(\beta; Q)$). The following bound holds:

$$\sup_{\beta \in \mathbb{R}^p} \|\nabla F^{KRR}_\lambda(\beta; Q)\|_\infty \leq \frac{1}{\lambda} \cdot |h'(0)| \cdot (2M_X)^q \cdot M_Y^2.$$ 

Proof This is Proposition 15 in Ruan et al. (2021). \[ \square \]

Lemma A.9 (Lipschitzness of $\beta \mapsto F^{KRR}_\lambda(\beta)$). The following bound holds for all $\beta, \beta'$:

$$|F^{KRR}_\lambda(\beta; Q) - F^{KRR}_\lambda(\beta'; Q)| \leq \frac{1}{\lambda} \cdot |h'(0)| \cdot (2M_X)^q \cdot M_Y^2 \cdot \|\beta - \beta'\|_1.$$ 

Proof This is a consequence of Lemma A.8 and Taylor’s intermediate theorem. \[ \square \]

Lemma A.10 (Lipschitzness of $\beta \mapsto (F^{KRR}_\lambda(0; Q) - F^{KRR}_\lambda(\beta; Q))^2$). It holds for all $\beta, \beta'$:

$$|(F^{KRR}_\lambda(0; Q) - F^{KRR}_\lambda(\beta; Q))^2 - (F^{KRR}_\lambda(0; Q) - F^{KRR}_\lambda(\beta'; Q))^2| \leq \frac{1}{2\lambda^2} \cdot |h'(0)| \cdot (2M_X)^q \cdot M_Y^4 \cdot \|\beta - \beta'\|_1.$$ 

Proof This is a consequence of Lemma A.9. Note that $F^{KRR}_\lambda(0; Q) \leq M_Y^2$. \[ \square \]
A.2 Special properties $q = 1$

A.2.1 Generic Bounds on the Gradient $\nabla F^K_{X}^{\text{KRR}}(\beta)$

Introduce the auxiliary function $\hat{\nabla} F^K_{X}^{\text{KRR}}(\beta)$ coordinate-wisely defined by

$$(\hat{\nabla} F^K_{X}^{\text{KRR}}(\beta))_j = -\frac{1}{\lambda} \cdot \mathbb{E}[z_{\beta;\lambda}(X;Y) z_{\beta;\lambda}(X';Y') h(\|X - X'\|_1, \beta + |X_j - X'_j|)]$$  \hfill (57)

We abuse notation and write $\partial_{\beta_j} F^K_{X}^{\text{KRR}}(\beta) := (\hat{\nabla} F^K_{X}^{\text{KRR}}(\beta))_j$. The following Lemma A.11 is a direct consequence of Lemma C.9 and Lemma C.10 in [Ruan et al., 2021].

**Lemma A.11 (Generic Bound).** Let $q = 1$. The following holds for all $\beta \in \mathbb{R}_+^p$ and $l \in [p]$:

$$\partial_{\beta_l} F^K_{X}^{\text{KRR}}(\beta; Q) \leq -\frac{1}{2 \lambda} \cdot \left(-\lambda \cdot \partial_{\beta_l} F^K_{X}^{\text{KRR}}(\beta; Q) - C \lambda^{1/2} (1 + \lambda^{1/2})\right).$$

Here the constant $C > 0$ depends only on $M_X, M_Y, M_{\mu}$ (and does not depend on $\beta$).

A.2.2 Specific Bounds on the Gradient $\nabla F^K_{X}^{\text{KRR}}(\beta)$

**Lemma A.12 (Main Effect).** Assume $X_l$ is a main effect signal: $\text{Var}_Q(\mathbb{E}_Q[Y|X_l]) \neq 0$. Fix $\lambda_0 > 0$. Then there exist $c, C > 0$ such that the following bound holds for all $\lambda \leq \lambda_0$:

$$\partial_{\beta_l} F^K_{X}^{\text{KRR}}(\beta; Q) \mid_{\beta = 0} \leq -\frac{1}{\lambda} \cdot (c - C \lambda^{1/2}).$$  \hfill (58)

The constants $c, C > 0$ depend only on $Q, \mu, \lambda_0 > 0$ (and does not rely on $\lambda$).

**Proof** By Lemma A.11 it suffices to prove that, for some constant $c > 0$,

$$\lambda \partial_{\beta_l} F^K_{X}^{\text{KRR}}(\beta) = \mathbb{E}_Q[YY'h(|X_l - X'_l|)] \geq c.$$  \hfill (59)

As $X_l$ is a main effect, we know that $U(X_l) := \mathbb{E}[Y|X_l] \neq 0$. Consequently, we obtain

$$\mathbb{E}_Q[YY'h(|X_l - X'_l|)] = \mathbb{E}_Q[U(X_l)U(X'_l)h(|X_l - X'_l|)] > 0$$

where the last inequality uses the fact that $h$ is positive definite. \hfill $\square$

**Lemma A.13 (Conditional Main Effect).** Assume $X_l$ is a conditional main effect signal with respect to $X_T$: $\mathbb{E}_Q[Y|X_T] \neq \mathbb{E}_Q[Y|X_T\cup\{l\}]$. Fix $\lambda_0, \tau > 0$. Let $\beta^{0:T}$ be the vector where $\beta^0_T = \tau 1_T$ and $\beta^0_{Tc} = 0$. Then there exist $c, C > 0$ such that the bound below holds when $\lambda \leq \lambda_0$:

$$\partial_{\beta_l} F^K_{X}^{\text{KRR}}(\beta; Q) \mid_{\beta = \beta^{0:T}} \leq -\frac{1}{\lambda} \cdot (c - C \lambda^{1/2}),$$  \hfill (59)

where the constants $c$ and $C > 0$ depend only on $Q, \mu, \lambda_0, \tau > 0$ (and do not depend on $\lambda$).
**Proof** For notational simplicity, we write \( Z = z_{\beta, \lambda}(X; Y) \mid_{\beta = \beta_0, T} \) and write \( \hat{\beta} \) to be the vector which has the same coordinates as \( \beta_0, T \) except at \( l \) where \( \hat{\beta}_l = 1 \). By Lemma A.11, it suffices to prove that, for some constant \( c > 0 \),

\[
\lambda \hat{\beta} \mathcal{F}_{\lambda}^{\text{KRR}}(\beta) \mid_{\beta = \beta_0, T} = \mathbb{E}_Q[ZZ'h(\|X - X'\|_{1, \hat{\beta}})] \geq c.
\]

Now, \( X_l \) is a conditional main effect with respect to \( X_T \) by assumption. Hence, we obtain

\[
\mathbb{E}_Q[Z | X_T \cup \{l\}] := \mathbb{E}_Q[Z | X_T \cup \{l\}] \neq 0.
\]

Consequently, we obtain the inequality

\[
\mathbb{E}_Q[ZZ'h(\|X - X'\|_{1, \hat{\beta}})] = \mathbb{E}_Q[U(X_T \cup \{l\})U(X_T' \cup \{l\})h(\|X - X'\|_{1, \hat{\beta}})] > 0,
\]

where the last inequality uses the fact that \( h \) is positive definite.

\[\square\]

## B Basics on Differential Inclusions

This section reviews basic results on differential inclusions, and in particular the gradient inclusions. Our definitions and notation follow closely the standard references [Aubin and Cellina (2012)].

**Definition B.1** (Differential Inclusion ([Aubin and Cellina (2012)])). The differential inclusion associated with the set-valued mapping \( G : \mathbb{R}^p \rightrightarrows \mathbb{R}^p \) from the point \( x_0 \in \mathbb{R}^p \) denoted by

\[
\dot{x} \in G(x), \quad x(0) = x_0
\]

is defined by any absolutely continuous function \( x : U \to \mathbb{R}^p \) satisfying for all \( t \in U \)

\[
x(t) = x_0 + \int_0^t v(s)ds,
\]

where \( v : \mathbb{R}_+ \to \mathbb{R}^p \) is some measurable function satisfying \( v(s) \in G(x(s)) \) for all \( s \in U \).

Our focus is on the gradient inclusion. We restrict the objective functions to be weakly convex functions, whose definition is given below.

**Definition B.2.** A function \( f : \mathbb{R}^p \to \mathbb{R} \cup \{\infty\} \) is called weakly convex if there exists \( \lambda \geq 0 \) such that the function \( f(x) + \frac{\lambda}{2} \|x\|^2 \) is convex.

All the objective functions considered in this paper are weakly convex (Example 4).

**Example 4:** A convex function \( f \) is a weakly convex function. A function \( f \) with domain convex on which the gradient is Lipschitz is a weakly convex function. ♦

Let \( f \) be a weakly convex function and \( X \) be a closed convex set. Consider

\[
\min_{x \in X} f(x).
\]

The associated gradient inclusion is given by

\[
\dot{x}(t) \in -\partial f(x) - N_X(x) \quad \text{and} \quad x(0) = x_0.
\] (60)

Theorem 4 establishes the existence, uniqueness, and monotonicity of the solution of the gradient inclusion (60). The proof is standard (see, e.g., [Duchi and Ruan (2018) Theorem 3.15]).
**Theorem 4** (Existence, Uniqueness, Monotonicity of the Solution of the Gradient Inclusion). Assume the function $f$ is closed and weakly convex. Let $X$ be a closed convex set with $X \subseteq \text{dom}(f)$. Assume $f(x) + \mathbb{I}_X(x)$ is coercive: $\lim_{x \to \infty} f(x) + \mathbb{I}_X(x) = \infty$. Then for any $x_0 \in X$, there is a unique solution $x$ of the differential inclusion \(^{[60]}\) defined on $\mathbb{R}_+$. The solution satisfies the properties (i) $x(t) \in X$, (ii) $x(t)$ is Lipschitz in $t$, and (iii)

$$f(x(t)) \leq f(x(0)) - \int_0^t \|g^*(x(s))\|_2^2 \, ds \quad \text{for all } t \in \mathbb{R}_+.$$ 

We define $g^*(x) : X \mapsto \mathbb{R}^p$ is defined by $g^*(x) = \text{argmin}\{\|g\|_2 : g \in \partial f(x) + \mathcal{N}_X(x)\}$.

The differential inclusion has benign stability guarantees when it is a Lipschitz differential inclusion. We say that the mapping $G : \mathbb{R}^p \rightrightarrows \mathbb{R}^p$ is $L$-Lipschitz if $\text{dist}(G(x), G(y)) \leq L \|x - y\|_2$ for all $x, y \in \mathbb{R}^p$, where $\text{dist}(G_1, G_2) := \inf_{g_1 \in G_1, g_2 \in G_2} \|g_1 - g_2\|_2$.

**Example 5:** Let $X$ be a closed convex set. Let $f$ be a function which is $L$-Lipschitz on $X$ and which satisfies $f(x) = 0$ for all $x \notin X$. Consider the set-valued mapping $G(x) = f(x) + \mathcal{N}_X(x)$ which is defined on $\mathbb{R}^p$. Then $G : \mathbb{R}^p \rightrightarrows \mathbb{R}^p$ is $L$-Lipschitz. \(\blacklozenge\)

The following result concerns the stability of Lipschitz differential inclusion. We say that the mapping $G$ is outer-semicontinuous if for any sequence $x_n \to x \in \text{dom}(G)$, we have the inclusion $\limsup_{n \to \infty} G(x_n) \subseteq G(x)$. Here the limit supremum for a sequence of sets $A_n \subseteq \mathbb{R}^p$, is defined by $\limsup_{n} A_n = \{y : \exists y_{n_k} \in A_{n_k}, y_{n_k} \to y \text{ as } k \to \infty\}$. Note that the gradient mapping $G(x) = -\partial f(x) - \mathcal{N}_X(x)$ that appears in the right-hand side of Eq. \(^{[60]}\) is outer-semicontinuous (see, e.g., Duchi and Ruan [2018], Lemma 3.6).

**Theorem 5** (Grönewall inequality of Lipschitz Differential Inclusion \(^{[Aubin and Cellina 2012]}\)). Let $G : \mathbb{R}^p \rightrightarrows \mathbb{R}^p$ and $\tilde{G} : \mathbb{R}^p \rightrightarrows \mathbb{R}^p$ be non-empty, closed convex-valued, and outer-semicontinuous. Consider the two differential inclusions $x, \tilde{x}$ associated with the set-valued mapping $G, \tilde{G}$:

\[
\begin{align*}
\dot{x} &= G(x), \quad x(0) = x_0. \\
\dot{\tilde{x}} &= \tilde{G}(\tilde{x}), \quad \tilde{x}(0) = x_0.
\end{align*}
\]

Assume (i) $G$ is $L$-Lipschitz set-valued mapping, (ii) $\sup_{x \in \mathbb{R}^p} \text{dist}(G(x), \tilde{G}(x)) = \Delta < \infty$ and (iii) there exists a solution $x$ for the inclusion \(^{[61]}\) on the interval $[0, T]$. Then there exists a solution $\tilde{x}$ for the inclusion \(^{[62]}\) on the interval $[0, T]$ which satisfies

\[
\sup_{t \in [0, T]} \|\tilde{x}(t) - x(t)\|_2 \leq \frac{\Delta}{L} \cdot e^{LT}.
\]

### C Deferred Technical Proofs

#### C.1 Details of the proof of Theorem 3

This section continues the proof of Theorem 3.
We start by considering the case where $\beta_{S^c} = 0$, and show that the desired gradient lower bound \cite{23} in the statement of Theorem \cite{3} holds for all $\beta$ such that $\beta_{S^c} = 0$. Fix a noise variable $j \notin S$. Substituting Eq. \cite{24} into Eq. \cite{32} yields for $j \notin S$

$$
\partial_{\beta_j} F^{\text{KRR}}_\lambda (\beta; \mathbb{Q}) = \frac{1}{\lambda} \int_0^\infty \mathbb{E}_Q \left[ z_{\beta;\lambda}(X;Y) z_{\beta;\lambda}(X';Y') t e^{-t\|X-X'||_{q,\beta}^q} | X_j - X'_j |^q \right] \mu(dt). \quad (64)
$$

We analyze the integrand on the right-hand side. As $\beta_{S^c} = 0$, $\mathbb{E}[z_{\beta;\lambda}(X;Y)|X] = f^*(X_S) - f_{\beta,\lambda}(\beta^{1/q} \circ X)$ is a function only of the signal variable $X_S$, and similarly, $e^{-t\|X-X'||_{q,\beta}^q}$ is a function only of $X_S$, too. As $X_S \perp X_{S^c}$, we can decompose the integrand on the right-hand side into:

$$
\mathbb{E}_Q \left[ z_{\beta;\lambda}(X;Y) z_{\beta;\lambda}(X';Y') t e^{-t\|X-X'||_{q,\beta}^q} | X_j - X'_j |^q \right] = \mathbb{E}_Q \left[ z_{\beta;\lambda}(X;Y) z_{\beta;\lambda}(X';Y') t e^{-t\|X-X'||_{q,\beta}^q} \right] \cdot \mathbb{E}_Q \left[ |X_j - X'_j |^q \right]. \quad (65)
$$

Substitute Eq. \cite{65} back into Eq. \cite{64}. We obtain for all $\beta$ such that $\beta_{S^c} = 0$

$$
\partial_{\beta_j} F^{\text{KRR}}_\lambda (\beta; \mathbb{Q}) = \frac{1}{\lambda} \int_0^\infty \mathbb{E}_Q \left[ z_{\beta;\lambda}(X;Y) z_{\beta;\lambda}(X';Y') t e^{-t\|X-X'||_{q,\beta}^q} \right] \mu(dt) \cdot \mathbb{E}_Q \left[ |X_j - X'_j |^q \right]. \quad (66)
$$

Since the following integral representation of the kernel function holds

$$
h(\|X-X'||_{q,\beta}^q) = \int_0^\infty e^{-t\|X-X'||_{q,\beta}^q} \mu(dt), \quad (67)
$$

we can use the assumption that $\text{supp}(\mu) \subseteq [m_\mu, M_\mu]$ where $0 < m_\mu < M_\mu < \infty$ and apply the Markov’s inequality to Eq. \cite{66} to conclude that for all $\beta$ such that $\beta_{S^c} = 0$

$$
\partial_{\beta_j} F^{\text{KRR}}_\lambda (\beta; \mathbb{Q}) \geq \frac{1}{\lambda} \cdot m_\mu \cdot \mathbb{E}_Q \left[ z_{\beta;\lambda}(X;Y) z_{\beta;\lambda}(X';Y') h(\|X-X'||_{q,\beta}^q) \right] \cdot \mathbb{E}_Q \left[ |X_j - X'_j |^q \right]. \quad (68)
$$

To finalize the proof of the desired gradient lower bound \cite{23} for all the $\beta$ where $\beta_{S^c} = 0$, we invoke Lemma \ref{A.2} and Lemma \ref{A.4}. Lemma \ref{A.2} itself is of crucial importance because it builds a non-trivial identity that connects the regressor $f_{\beta,\lambda}$ and the residual $z_{\beta;\lambda}$:

$$
\mathbb{E}_Q \left[ z_{\beta;\lambda}(X;Y) z_{\beta;\lambda}(X';Y') h(\|X-X'||_{q,\beta}^q) \right] = \lambda^2 \|f_{\beta,\lambda}\|^2_H, \quad (69)
$$

where above $f_{\beta,\lambda}$ denotes the minimum of the kernel ridge regression indexed by $\beta$, i.e.,

$$
f_{\beta,\lambda} = \arg\min_{f \in \mathcal{H}} \frac{1}{2} \mathbb{E}_Q \left[ (Y - f(\beta^{1/q} \circ X))^2 \right] + \frac{\lambda}{2} \|f\|^2_H. \quad (70)
$$

Lemma \ref{A.4} further lower bounds the Hilbert norm of the fitted regression function $f_{\beta,\lambda}$ in terms of the deviation of the objective value from $F^{\text{KRR}}_\lambda (\beta; \mathbb{Q})$ to $F^{\text{KRR}}_\lambda (0; \mathbb{Q})$:

$$
\|f_{\beta,\lambda}\|^2_H \geq \frac{1}{|h(0)| M_\mu^2} \cdot (F^{\text{KRR}}_\lambda (0; \mathbb{Q}) - F^{\text{KRR}}_\lambda (\beta; \mathbb{Q}))^2. \quad (70)
$$
Substitute equations (69)–(70) into inequality (68). This shows for all $\beta$ where $\beta_{S^c} = 0$,

$$
\partial_j F_\lambda^{KRR}(\beta; \mathbb{Q}) \geq c_j \cdot \lambda \left( F_\lambda^{KRR}(0; \mathbb{Q}) - F_\lambda^{KRR}(\beta; \mathbb{Q}) \right)_+^2,
$$

where $c_j = \frac{m_\mu}{|h(0)| M_Y^2} \cdot \mathbb{E}_Q [ |X_j - X_j'| ]$.

This gives the desired gradient lower bound for the $\beta$ when $\beta_{S^c} = 0$.

Next, we extend the gradient lower bound to the general case where we do not put any restriction on $\beta$. The key mathematical result that allows this is Lemma A.7 and Lemma A.10 where it is shown that the following two mappings are Lipschitz on $\mathbb{R}_+^p$

$$
\beta \mapsto \partial_{\beta_j} F_\lambda^{KRR}(\beta; \mathbb{Q}), \quad \text{and} \quad \beta \mapsto \lambda(F_\lambda^{KRR}(0; \mathbb{Q}) - F_\lambda^{KRR}(\beta; \mathbb{Q}))_+^2.
$$

with the Lipschitz constants bounded by $C_1(1 + \lambda)/\lambda^2$ and $C_2$, where $C_1, C_2$ are constants that depend only on $M_X, M_Y, \mu$. As a direct consequence of this fact, the general gradient lower bound (23) follows immediately from the special lower bound that we have established in Eq. (71). Formally, for any $\beta \in \mathbb{R}_+^p$, we construct a surrogate $\beta'$ such that they differ only on the noise coordinates: $\beta'_S = \beta_S$ and $\beta'_{S^c} = 0$. We first apply the special gradient lower bound to the surrogate $\beta'$ (where $\beta'_{S^c} = 0$)

$$
\partial_{\beta_j} F_\lambda^{KRR}(\beta'; \mathbb{Q}) \geq c_j \cdot \lambda \left( F_\lambda^{KRR}(0; \mathbb{Q}) - F_\lambda^{KRR}(\beta'; \mathbb{Q}) \right)_+^2,
$$

and then using the Lipschitzness of the mappings in Eq. (72), we obtain

$$
\partial_{\beta} F_\lambda^{KRR}(\beta; \mathbb{Q}) \geq \partial_{\beta_j} F_\lambda^{KRR}(\beta'; \mathbb{Q}) - C_1 \cdot \frac{1 + \lambda}{\lambda^2} \cdot \|\beta_{S^c}\|_1
$$

$$
\lambda \left( F_\lambda^{KRR}(0; \mathbb{Q}) - F_\lambda^{KRR}(\beta'; \mathbb{Q}) \right)_+^2 \geq \lambda \left( F_\lambda^{KRR}(0; \mathbb{Q}) - F_\lambda^{KRR}(\beta; \mathbb{Q}) \right)_+^2 - C_2 \|\beta_{S^c}\|_1
$$

Now we can combine the two inequalities in Eq. (73) and Eq. (74) to derive the final gradient lower bound that holds for all $\beta$ (with some appropriate $M$)

$$
\partial_{\beta_j} F_\lambda^{KRR}(\beta; \mathbb{Q}) \geq c_j \cdot \lambda \left( F_\lambda^{KRR}(0; \mathbb{Q}) - F_\lambda^{KRR}(\beta; \mathbb{Q}) \right)_+^2 - C \cdot \frac{1 + \lambda^2}{\lambda^2} \|\beta_{S^c}\|_1.
$$

C.2 Proof of Proposition 1B

The proof is similar to that of Proposition 1A. Note that $B^*$ consists only of the global minimum $\beta^*$ of the non-negative garrotte. Fix a noise variable $j \not\in S$. We show that

$$
\lim_{\beta \rightarrow \beta^*} \text{sign}(\beta_j) \cdot \partial_{\beta_j} F_\gamma^{NG}(\beta; \mathbb{Q}) = \gamma.
$$

Denote $z_{\beta;\lambda}(X; Y) = Y - \sum_{i=1}^p w_i \beta_i X_i$ to be the residual, where we recall that $w_i$ is the solution of the ordinary least square between $Y$ and $X$. At any $\beta$,

$$
\text{sign}(\beta_j) \cdot \partial_{\beta_j} F_\gamma^{NG}(\beta; \mathbb{Q}) = \gamma - \text{sign}(\beta_j) \cdot w_j \cdot \mathbb{E}_Q \left[ X_j z_{\beta;\lambda}(X; Y) \right].
$$

Note $\lim_{\beta \rightarrow \beta^*} \mathbb{E}_Q \left[ X_j z_{\beta;\lambda}(X; Y) \right] = \mathbb{E}_Q \left[ X_j r_{\beta^*}(X; Y) \right] = \text{Cov}_Q(X_j, r_{\beta^*}(X; Y)) = 0$ where the second identity uses (i) $\text{supp}(\beta^*) \subseteq S$, (ii) $\mathbb{E}[Y | X] = \mathbb{E}[Y | X_S]$ and (iii) $X_S \perp X_{S^c}$.

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\section*{C.3 Proof of Proposition 1C}

We compute the gradient of the objective $F_{\lambda,\gamma}^{\text{LIN}}(\beta; Q)$ with respect to $\beta$. Applying the envelope theorem, we obtain the following expression that holds for all coordinate $j \in [p]$

$$\partial_{\beta_j} F_{\lambda,\gamma}^{\text{LIN}}(\beta; Q) = \gamma - \mathbb{E}_Q[X_j z_{\beta,\lambda}(X; Y)],$$

where $z_{\beta,\lambda}(X; Y) = Y - \sum_{i=1}^p \beta_i w_i(\beta) X_i$ denotes the residual, where $w^*(\beta)$ is the solution

$$w^*(\beta) = \arg\min_w \frac{1}{2} \mathbb{E}_Q[(Y - \sum_{i=1}^p \beta_i w_i X_i)^2] + \frac{\lambda}{2} \|w\|^2.$$

Note $w_j^*(\beta) = 0$ for all $j \notin S$ since (i) $\mathbb{E}[Y|X] = \mathbb{E}[Y|X_S]$ and (ii) $X_S \perp X_{S^c}$. Hence, $\mathbb{E}_Q[z_{\beta,\lambda}(X; Y)|X] = X_j$ for any variable $j \notin S$. As a result, we obtain $\mathbb{E}_Q[X_j z_{\beta,\lambda}(X; Y)] = 0$ for all $j \notin S$ and for all $\beta$. This proves in particular that for all $j \notin S$, and for all $\beta$,

$$\text{sign}(\beta_j) \cdot \partial_{\beta_j} F_{\lambda,\gamma}^{\text{LIN}}(\beta; Q) = \gamma. \quad (78)$$

Hence, the objective $F_{\lambda,\gamma}^{\text{LIN}}(\beta; Q)$ is self-penalizing if and only if $\gamma > 0$.

\section*{C.4 Proof of Proposition 3}

The proof is based on standard approximation-theoretic arguments.

The key to the proof is to show that $\mathcal{H}$ is a universal RKHS (Micchelli et al., 2006). Write the kernel in terms of $v(x - x') = h(||x - x'||_q^q)$. The characterization of $h$ in Eq. (11) gives

$$v(z) = \int_0^\infty e^{-t||z||_q^q} \mu(dt). \quad (79)$$

According to (Micchelli et al., 2006) Proposition 15), $\mathcal{H}$ is universal if the Fourier transform of $v$ has full support. With the expression (79), we can easily show that the Fourier transform $\mathcal{F}(v)$ is

$$\mathcal{F}(v)(\omega) = (2\pi)^{p/2} \cdot \int_0^\infty \prod_{i=1}^p \frac{1}{t^{1/q}} \theta \left( \frac{\omega}{t^{1/q}} \right) \mu(dt) \quad (80)$$

where $\theta(\omega) = 1/(1 + \omega^2)$ when $q = 1$ and $\theta(\omega) = e^{-\omega^2/4}/2\sqrt{\pi}$ when $q = 2$. As $\theta$ has full support, expression (80) shows that $\mathcal{F}(v)$ has full support, and hence $\mathcal{H}$ is universal.

The universal approximation property of the universal RKHS $\mathcal{H}$ implies that for any compact set $\mathcal{W}$, any continuous function $f$ on $\mathcal{W}$ and $\epsilon > 0$, there exists a function $g \in \mathcal{H}$ such that $\sup_{x \in \mathcal{W}} |f(x) - g(x)| \leq \epsilon$ (Micchelli et al., 2006). Consequently, the universal approximating property implies that for any $\epsilon > 0$, there exists a function $f \in \mathcal{H}$ such that

$$\mathbb{E}_Q \left[ (\mathbb{E}[Y|X_{\text{supp}(\beta)}] - \bar{f}(\beta^{1/q} \circ X))^2 \right] \leq \epsilon. \quad (81)$$

We can take $\lambda$ sufficiently small, say $\lambda \leq \lambda_0$ so that $\lambda \|\bar{f}\|^2_{\mathcal{H}} \leq \epsilon$. Consequently, the ANOVA decomposition and triangle inequality lead to the following bound that holds for all $\lambda \leq \lambda_0$:

$$F_{\lambda}^{\text{KRR}}(\beta; Q) \leq \frac{1}{2} \mathbb{E}[(Y - \bar{f}(\beta^{1/q} \circ X))^2] + \frac{\lambda}{2} \|\bar{f}\|^2_{\mathcal{H}} \leq \frac{1}{2} \mathbb{E}[\text{Var}(Y|X_{\text{supp}(\beta)})] + \epsilon. \quad (82)$$

This immediately leads to Proposition 3 as desired.
C.5 Proof of Lemma 5.2

Lemma 5.2 is a mere consequence of the following two components: (i) the Lyapunov convergence theorem for the gradient inclusion and (ii) a lower bound on the size of the gradient at the beginning stage of the differential inclusion. In below discussions, we use \(C_1, C_2, \ldots\) to denote constants that does not depend on \(\lambda, n\).

Formally, according to the Lyapunov theorem (Theorem 4), we have for all \(t \geq 0\):
\[
F^\text{KRR}_\lambda(\beta(t); \mathcal{Q}) \leq F^\text{KRR}_\lambda(\beta(0); \mathcal{Q}) - \int_0^t \|g^⋆(\beta(s))\|_2^2 \, ds,
\]
(83)
where the mapping \(g^⋆(\beta) := \arg\min \{\|g\|_2 : g \in \nabla F^\text{KRR}_\lambda(\beta; \mathcal{Q}) + N_{\mathcal{Z}}(\beta)\}\) denotes the minimal gradient at each \(\beta \in \mathcal{Z}\). In words, the theorem says that the objective value has a certain rate of decay governed by the minimal size of the gradient along the trajectory.

Lemma A.6 and Lemma C.2 give the following formula of the gradient at \(\beta(0) = 0\). For each coordinate \(j \in [p]\), the gradient of the objective has the following expression:
\[
\partial_\beta F^\text{KRR}_\lambda(0; \mathcal{Q}) = \frac{1}{\lambda} |h'(0)| E_Q[Y Y' (X_j - X_j)^2] = \frac{1}{\lambda} |h'(0)| \int_0^\infty |E_Q[Y e^{i\omega X_j}]|^2 \cdot \frac{d\omega}{\pi \omega^2}.
\]
(84)
Note the integral is positive \(\int_0^\infty |E_Q[Y e^{i\omega X_j}]|^2 \cdot \frac{d\omega}{\pi \omega^2} > 0\) whenever \(\text{Var}_Q(E_Q[Y|X_j]) \neq 0\). As its consequence, the following lower bound holds for some constant \(C_1\):
\[
\|g^⋆(\beta(0))\|_2 = \|g^⋆(0)\|_2 \geq -\partial_\beta F^\text{KRR}_\lambda(0; \mathcal{Q}) \geq \frac{1}{\lambda} \cdot C_1.
\]
(85)
Below we extend the bound (85) to \(\|g^⋆(\beta(t))\|_2\) for small \(t > 0\) by exploiting the Lipschitz-ness of the mapping \(t \mapsto \|g^⋆(\beta(t))\|_2\) near \(t = 0\). Note the following facts.

(i) The trajectory \(t \mapsto \beta(t)\) is \(C_2/\lambda\) Lipschitz as the gradient \(\nabla F^\text{KRR}_\lambda(\beta; \mathcal{Q})\) is uniformly bounded in the feasible set \(\mathcal{Z}\) (Lemma A.8).

(ii) The gradient mapping \(\beta \mapsto \nabla F^\text{KRR}_\lambda(\beta; \mathcal{Q})\) is \(C_3/\lambda^2\) Lipschitz.

The composition rule gives that \(t \mapsto \nabla F^\text{KRR}_\lambda(\beta(t); \mathcal{Q})\) is also Lipschitz with the constant \(M_3 = C_4/\lambda^3\) where \(C_4 = C_2 C_3\). Consequently, this implies the lower bound \(\|g^⋆(\beta(t))\|_2 \geq \frac{1}{2} \|g^⋆(\beta(0))\|_2 \geq \frac{1}{2\lambda} \cdot C_1\) when \(t \leq C_5 \lambda^2\) for sufficiently small \(C_5\). As a consequence, we can now apply Lyapunov theorem (83) to obtain for \(C_6 = C_1^2 C_5/4\)
\[
F^\text{KRR}_\lambda(\beta(t); \mathcal{Q}) \leq F^\text{KRR}_\lambda(\beta(0); \mathcal{Q}) - C_6 \quad \text{when } t = C_5 \lambda^2.
\]
(86)

C.6 Proof of Proposition 7

We prove the result accordingly in the three bullet points below.

- The first point follows from Lemma 5.2. Lemma 5.2 shows that
\[
F^\text{KRR}_\lambda(\beta(t); \mathcal{Q}) \leq F^\text{KRR}_\lambda(\beta(0); \mathcal{Q}) - 3c \quad \text{when } t = C \lambda^2.
\]
where \(c, C > 0\) do not depend on \(n, \lambda\). The self-penalizing property implies \(\|\beta_{S^c}(t)\|_1 = 0\) for \(t \geq 0\). This implies that the gradient dynamic enters \(\mathcal{X}_{3c, \delta', \lambda}\) at time \(t = C \lambda^2\) for any \(\delta' > 0\). The inclusion \(\mathcal{X}_{3c, \delta'/81 \lambda} \subseteq \mathcal{X}_{c, \delta, \lambda}\) simply holds according to the definition.
• The second point is simply a restatement of the self-penalizing property of the kernel ridge regression objective (Corollary 4.2).

• The third point follows from the self-penalizing property of $\mathcal{X}_{c,\delta,\lambda}$ and the monotonicity of the gradient dynamics. Indeed, any gradient dynamics initiated from $\mathcal{X}_{c,\delta,\lambda}$ must (i) monotonically decrease the objective values by Theorem 3 (ii) monotonically decrease the size of the noise variables as the objective is self-penalizing on the set $\mathcal{X}_{c,\delta,\lambda}$. This proves invariance of $\mathcal{X}_{c,\delta,\lambda}$.

C.7 Proof of Proposition 7

Proposition 7 is almost an immediate consequence of the population version, i.e., Proposition 4. Let $c, C, \delta > 0$ be the constant such that Proposition 4 holds. The following fact is used throughout the proof, which follows from triangle inequality and definition of $\Omega_n$:

$$\mathcal{X}_{3c,\delta/81,\lambda,n} \subseteq \bar{\mathcal{X}}_{2c,\delta/16,\lambda,n} \subseteq \mathcal{X}_{c,\delta,\lambda,n} \text{ on the event } \Omega_n(c).$$

Below we set $\bar{c} = 2c$, $\bar{C} = C$, $\bar{\delta} = \delta/16$, $\bar{\delta} = \delta$. Let $\epsilon \leq c$ so that $\Omega_n(\epsilon \lambda) \subseteq \Omega_n(c)$ as $\lambda \leq 1$.

We shall determine the constant $c \geq \epsilon > 0$ as the minimum of $\epsilon_1, \epsilon_2$ where $\epsilon_1, \epsilon_2 > 0$ are given in the first and second bullet point below. Noticeably, the constants $\epsilon_1, \epsilon_2 > 0$ thus defined are independent of $\lambda, n$.

• Below we prove that $\bar{\beta}(t) \in \bar{\mathcal{X}}_{c,\delta,\lambda,n}$ at time $t = \bar{C}\lambda^2$ on event $\Omega_n(\epsilon_1 \lambda)$ where $\epsilon_1 > 0$ is determined below. By Proposition 7, $\beta(t) \in \mathcal{X}_{c,\delta/81,\lambda,n}$ at time $t = C\lambda^2$, i.e.,

$$\|\beta_S^c(t)\|_1 \leq c^2\delta\lambda^3/9 \text{ and } F_{\lambda}^{\text{KRR}}(\beta(t); Q) < F_{\lambda}^{\text{KRR}}(0; Q) - 3c \text{ for } t = C\lambda^2. \quad (88)$$

By Lemma C.1, we can pick $c/2 > \epsilon_1 > 0$ small enough such that on event $\Omega_n(\epsilon_1 \lambda)$:

$$\|\bar{\beta}(t) - \beta(t)\|_1 \leq c^2\delta\lambda^3/9 \text{ and } |F_{\lambda}^{\text{KRR}}(\beta(t); Q) - F_{\lambda}^{\text{KRR}}(\bar{\beta}(t); Q_n)| \leq c/2 \text{ for } t \leq C\lambda^2. \quad (89)$$

Now the triangle inequality gives the following bound on the event $\Omega_n(\epsilon_1 \lambda)$:

$$\|\bar{\beta}_S^c(t)\|_1 \leq c^2\delta\lambda^3/4 \text{ and } F_{\lambda}^{\text{KRR}}(\bar{\beta}(t); Q_n) < F_{\lambda}^{\text{KRR}}(0; Q_n) - 2c \text{ for } t = C\lambda^2. \quad (90)$$

In other words, this says that $\tilde{\beta}(t) \in \bar{\mathcal{X}}_{c,\delta,\lambda,n}$ at time $t = \bar{C}\lambda^2$.

• The objective is self-penalizing on the set $\bar{\mathcal{X}}_{c,\delta,\lambda,n}$ on the event $\Omega_n(\epsilon_2 \lambda)$ where $0 < \epsilon_2 \leq c$ is determined below. Proposition 4 says that $F_{\lambda}^{\text{KRR}}(\beta; Q)$ is self-penalizing on the set $\mathcal{X}_{c,\delta,\lambda}$. This means that the population gradient $\partial_{\beta} F_{\lambda}^{\text{KRR}}(\beta; Q)$ has a uniform lower bound over the set of $\beta \in \mathcal{X}_{c,\delta,\lambda}$ and the set of noise variables $j \not\in S$. A careful traceback of the proof shows that the lower bound can be taken as $\epsilon_2 \lambda$ (Theorem 3) where $\epsilon$ is some constant that’s independent of $n, \lambda$.

Now we pick $\epsilon_2 = \epsilon/2 \wedge c$ and consider the event $\Omega_n(\epsilon_2 \lambda)$. On the event $\Omega_n(\epsilon_2 \lambda)$, by triangle inequality, the empirical gradient $\partial_{\beta} F_{\lambda}^{\text{KRR}}(\beta; Q_n)$ has a uniform lower bound $\epsilon_2 \lambda/2 > 0$ over $\beta \in \mathcal{X}_{c,\delta,\lambda}$ and $j \not\in S$. Note the exactly same lower bound also holds over $\beta \in \bar{\mathcal{X}}_{c,\delta,\lambda,n}$ since the inclusion $\bar{\mathcal{X}}_{c,\delta,\lambda,n} \subseteq \mathcal{X}_{c,\delta,\lambda}$ holds on the event $\Omega_n(\epsilon_2 \lambda)$. 

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• The set $\tilde{X}_{\epsilon, \delta, \lambda, n}$ is invariant with respect to the gradient dynamics of $F^{\text{KRR}}(\cdot; Q_n)$ on the event $\Omega_n(\epsilon \lambda)$ where $\epsilon = \epsilon_1 \land \epsilon_2$. This follows from the self-penalizing property of $\tilde{X}_{\epsilon, \delta, \lambda, n}$ and the monotonicity of the gradient dynamics. Indeed, any gradient dynamics initiated from $\tilde{X}_{\epsilon, \delta, \lambda, n}$ must (i) monotonically decrease the objective values by Theorem 4 (ii) monotonically decrease the size of the noise coordinates as the objective is self-penalizing on the set $\tilde{X}_{\epsilon, \delta, \lambda, n}$. This proves the invariance of $\tilde{X}_{\epsilon, \delta, \lambda, n}$ on $\Omega_n(\epsilon_2 \lambda)$.

As a consequence, there exists $\tau < \infty$ so that $\emptyset \subset \supp(\beta(t)) \subset S$ for all $t \geq \tau$ on the event $\Omega_n(\epsilon \lambda)$. Furthermore, we can choose the value of $\tau = \overline{\epsilon} \lambda^2$ where $\overline{\epsilon}$ is independent of $n, \lambda$ (since within the set $\tilde{X}_{\epsilon, \delta, \lambda, n}$ (i) the size of the noise variable is at most $c^2 \delta \lambda^3$ and (ii) the gradient with respect to the noise variables is at least $c \lambda/2$, and hence it takes at most $(2 c^2 \delta/\overline{\epsilon}) \cdot \lambda^2$ time for the gradient descent to move the noise variables to exactly 0).

Lemma C.1. Consider the population and empirical gradient flow $t \mapsto \beta(t)$ and $t \mapsto \tilde{\beta}(t)$ that share the same initializations $\beta(0) = \tilde{\beta}(0)$. Then there exists a constant $C > 0$ which does not depend on $n, \lambda$ such that for any $\epsilon > 0$, the deviation bound below holds on $\Omega_n(\epsilon)$:

$$\|\tilde{\beta}(t) - \beta(t)\|_1 \leq C \epsilon \lambda^2 \cdot e^{Ct/\lambda^2} \quad \text{for all } t \geq 0. \quad (91)$$

Moreover, the empirical and population objectives evaluated at its corresponding gradient flow has the following deviation bound on $\Omega_n(\epsilon)$.

$$\left| F^{\text{KRR}}_{\lambda}(\beta(t); Q) - F^{\text{KRR}}_{\lambda}(\tilde{\beta}(t); Q_n) \right| \leq \epsilon \lambda \epsilon \lambda \cdot e^{Ct/\lambda^2} \quad \text{for all } t \geq 0. \quad (92)$$

Proof Throughout the proof, we use $C_1, C_2, \ldots$, to denote constants independent of $n, \lambda$. The first point is a consequence of the Grönwall’s inequality in the theory of differential inclusion. On the event $\Omega_n(\epsilon)$, we have uniform control on the maximum $\ell_\infty$ deviations between the empirical and population gradient vector fields in the feasible set $Z$. Note that the population gradient field is Lipschitz in the following sense (see Proposition A.7):

$$\|\nabla F^{\text{KRR}}_{\lambda}(\beta; Q) - \nabla F^{\text{KRR}}_{\lambda}(\beta'; Q)\|_\infty \leq \frac{C_1}{\lambda^2} \cdot \|\beta - \beta'\|_1.$$

Viewing the empirical gradient flow as a perturbed version of the population gradient flow, the Grönwall's inequality (Theorem 5) yields the desired estimate in Eq. (91).

The second point follows from the uniform $\ell_\infty$ bound on the gradient and the $\ell_1$ deviation bound in Eq. (91). Formally, Lemma A.8 shows that $\|\nabla F^{\text{KRR}}_{\lambda}(\beta; Q)\|_\infty \leq C_2/\lambda$ holds for all $\beta$. With the $\ell_1$ bound in Eq. (91), Taylor’s intermediate theorem gives

$$\left| F^{\text{KRR}}_{\lambda}(\beta(t); Q) - F^{\text{KRR}}_{\lambda}(\tilde{\beta}(t); Q_n) \right| \leq C_3 \epsilon \lambda \cdot e^{Ct/\lambda^2} \quad \text{for all } t \geq 0.$$

Note $\left| F^{\text{KRR}}_{\lambda}(\tilde{\beta}(t); Q) - F^{\text{KRR}}_{\lambda}(\tilde{\beta}(t); Q_n) \right| \leq \epsilon$ for all $t \geq 0$ on the event $\Omega_n(\epsilon)$ by definition. By the triangle inequality, the desired estimate in Eq. (92) now simply follows. \qed
C.8 A technical lemma

Lemma C.2. Assume $X,Y$ are random variables such that $\mathbb{E}_Q[Y] = 0$ and $\mathbb{E}_Q[X^2] < \infty$. Let $(X',Y')$ be independent copies of $(X,Y)$. Then $\mathbb{E}_Q[Y Y'|X - X'|^q] \leq 0$ for $q = 1,2$.

Proof The lemma follows immediately from the following identities:

\begin{align}
\mathbb{E}_Q[Y Y'|X - X'|] &= -\int_0^\infty |\mathbb{E}_Q[\text{Cov}(Y,e^{i\omega X})]|^2 \cdot \frac{1}{\pi \omega^2} d\omega \\
\mathbb{E}_Q[Y Y'|X - X'|^2] &= -\text{Cov}_Q^2(Y,X).
\end{align}

(93)

The proof of Eq. (93) can be found in [Ruan et al., 2021, Section 3].

C.9 On the global minimum of the empirical metric learning objective

Proposition 10. Assume Assumptions 1 and 2. Assume $S \neq \emptyset$ and $S \subseteq \text{supp}(\beta(0))$. Then with probability at least $1 - \exp(-c'n)$, the global minimizer $\tilde{\beta}^*$ of the empirical metric learning objective $F_{\text{ML}}(\beta;Q_n)$ satisfies $\emptyset \subset \text{supp}(\tilde{\beta}^*) \subseteq S$. Here $c' > 0$ is independent of $n$.

Proof This is a consequence of Proposition 6' and Lemma 5.1. Indeed, Proposition 6' says that on some event $\Omega_n(\epsilon)$ where $\epsilon > 0$, the sublevel set $X_{c,n} = \{\beta \in \mathcal{Z} : F_{\text{ML}}(\beta;Q_n) < -c\}$ for some $c > 0$ is invariant and self-penalizing. As a result, the global minimizer, which belongs to the set $X_{c,n}$ must have support contained in the signal set $S$. Note then $\Omega_n(\epsilon)$ happens with probability at least $1 - \exp(-c'n)$ by Lemma 5.1.

D Concentration

This section presents a uniform concentration result for U-statistics. The result is particularly useful in showing the concentration of the objective values and gradients for the metric learning and for the kernel ridge regression (Section D.1 and D.2). The proof combines the idea of chaining standard in the empirical process theory [van der Vaart and Wellner, 2013] and a specific decoupling technique common in the analysis of U-statistics [Hoeffding, 1994].

To state the result, we introduce some notation. Let $U_\beta(z,z')$ be a family of U-statistics indexed by $\beta \in \mathcal{B}$. Let $H_\beta(Q) := \mathbb{E}_Q[U_\beta(Z,Z')]$ where $Z,Z'$ are independent copies sampled from the distribution $Q$. Let $Q_n$ denote the empirical distribution. Let $Q = \text{supp}(Q)$.

Proposition 11. Assume the following conditions. Let $||\cdot||$ be a norm on $\mathbb{R}^p$. Let $\alpha > 0$.

- Boundedness: $|U_\beta(z,z')| \leq M_Z$ for $\beta \in \mathcal{B}$ and $z,z' \in Q$.
- Hölder Continuity: $|U_\beta(z,z') - U_\beta'(z,z')| \leq L \|\beta - \beta'\|^\alpha$ for $\beta,\beta' \in \mathcal{B}$ and $z,z' \in Q$.
- Norm constraint: $\mathcal{B} \subseteq \{\beta : \|\beta\| \leq M\}$.

There exists a constant $C_\alpha$ depending only on $\alpha$ such that with probability at least $1 - e^{-t^2}$

$$
\sup_{\beta \in \mathcal{B}} |H_\beta(Q_n) - H_\beta(Q)| \leq \frac{C_\alpha}{\sqrt{n}} \cdot (ML\sqrt{p} + M_Z(1 + t)).
$$

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Proof Let $W \equiv \sup_{\beta \in \mathcal{B}} |H_\beta(Q_n) - H_\beta(Q)|$ denote the maximum deviation. We view $W \equiv W(Z_{1:n})$ as a function of the i.i.d. data $Z_{1:n} = (Z_1, Z_2, \ldots, Z_n)$. Clearly, the function is of bounded difference with bound $2M_Z/n$, i.e., for any $Z_{1:n}$ and $Z'_{1:n}$ differing in only one coordinate,

$$|W(Z_{1:n}) - W(Z'_{1:n})| \leq 2M_Z/n.$$  

McDiarmid’s inequality [McDiarmid, 1989] yields that with probability at least $1 - e^{-t^2}$:

$$W \leq \mathbb{E}[W] + \frac{2M_Z}{\sqrt{n}}t. \quad (94)$$

Below we bound $\mathbb{E}[W]$. Our major technique is the symmetrization argument followed by an upper bound on the Dudley’s metric entropy integral [van der Vaart and W, 2013]. Since the U-statistics $H_\beta(Q_n)$ is an average of dependent variables, we need to apply the decoupling technique due to Hoeffding before the symmetrization [Hoeffding, 1994]. Formally, introduce the following notation.

- Let $\Delta_\beta(z, z') = U_\beta(z, z') - \mathbb{E}[U_\beta(z, z')]$.
- Let $\sigma_{i,i'}$ be independent Radamacher random variables.
- The total index $\mathcal{I} = \{(i, i')|1 \leq i, i' \leq n\}$ can be divided into two groups: $\mathcal{I} = \mathcal{I}_+ \cup \mathcal{I}_0$ where $\mathcal{I}_+ = \{(i, i')|i \neq i', 1 \leq i, i' \leq n\}$ and $\mathcal{I}_0 = \{(i, i)|1 \leq i \leq n\}$. A simple combinatorial argument shows that we can further decompose $\mathcal{I}_+ = \bigcup_{j=1}^{J} \mathcal{I}_j$ where any two different tuple in the same $\mathcal{I}_j$ has no intersection—for any $(i_1, i_2), (i_3, i_4) \in \mathcal{I}_j$ we have $i_1 \neq i_2$ where $1 \leq l_1 < l_2 \leq 4$—and where $|\mathcal{I}_j| \geq \left\lfloor \frac{n}{2} \right\rfloor$ for all $1 \leq j \leq J$.

Now, we are ready to bound $\bar{W} = \mathbb{E}[W]$. As $\mathcal{I} = \bigcup_{j=0}^{J} \mathcal{I}_j$, we have

$$\bar{W} = \mathbb{E} \left[ \sup_{\beta \in \mathcal{B}} \frac{1}{n^2} \left| \sum_{(i, i') \in \mathcal{I}} \Delta_\beta(Z_i, Z'_{i}) \right| \right] \leq \sum_{j=0}^{J} \mathbb{E} \left[ \sup_{\beta \in \mathcal{B}} \frac{1}{n^2} \sum_{(i, i') \in \mathcal{I}_j} \Delta_\beta(Z_i, Z'_{i}) \right] = \sum_{j=0}^{J} \bar{W}_j$$

Now we bound each term $\bar{W}_j$ on the right-hand side. Use the boundedness assumption, it is easy to see that $\bar{W}_j \leq 2M_Z/n$ for all $j$. Below we give a tighter bound for $\bar{W}_j$ when $j \geq 1$.

The proof is based on the empirical process theory. Fix $j \geq 1$. By symmetrization, we obtain

$$\bar{W}_j \leq \frac{1}{n^2} \cdot \mathbb{E} \left[ \sup_{\beta \in \mathcal{B}} \sum_{(i, i') \in \mathcal{I}_j} \sigma_{i,i'} \Delta_\beta(Z_i, Z'_{i}) \right]. \quad (95)$$

Write $G_\beta = \sum_{(i, i') \in \mathcal{I}_j} \sigma_{i,i'} \Delta_\beta(Z_i, Z'_{i})$. Note then $\beta \mapsto G_\beta$ is continuous and $G_\beta - G_{\beta'}$ is subgaussian with parameter at most $\sqrt{nL} \| \beta - \beta' \|^2$. Dudley’s integral bound yields

$$\mathbb{E} \left[ \sup_{\beta \in \mathcal{B}} \sum_{(i, i') \in \mathcal{I}_j} \sigma_{i,i'} \Delta_\beta(Z_i, Z'_{i}) \right] \leq 12 \cdot \sqrt{nL} \cdot \int_0^\infty \sqrt{\log N(\mathcal{B}, \| \cdot \|, e^{1/\alpha})} \, dc, \quad (96)$$

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where \( N(\mathcal{B}, \|\cdot\|, \epsilon) \) is the covering number of the set \( \mathcal{B} \) using the \( \|\cdot\| \)-ball of radius \( \epsilon \). As \( \log N(\mathcal{B}, \|\cdot\|, \epsilon) = 0 \) for \( \epsilon > M \) and \( \log N(\mathcal{B}, \|\cdot\|, \epsilon) \leq p \log(3M/\epsilon) \) for \( \epsilon \leq M \), we obtain
\[
\int_0^\infty \sqrt{\log N(\mathcal{B}, \|\cdot\|, \epsilon^{1/\alpha})} d\epsilon \leq (3M)^{\alpha} \sqrt{p} \cdot \int_0^{1/3} \epsilon^{\alpha-1} \sqrt{\log(1/\epsilon)} d\epsilon. \tag{97}
\]

Consequently, we use equations (95)–(113) to obtain that \( W_j \leq C_\alpha M^\alpha L \sqrt{p/n}^{3/2} \) for \( j \geq 1 \), where \( C_\alpha = 12 \cdot 3^{\alpha} \int_0^{1/3} \epsilon^{\alpha-1} \sqrt{\log(1/\epsilon)} d\epsilon < \infty \). This in turn implies the bound on \( W \):
\[
W = W_0 + \sum_{j=1}^J W_j \leq C_\alpha \cdot \left( \frac{M \bar{Z}}{n} + M^\alpha L \cdot \sqrt{\frac{p}{n}} \right). \tag{98}
\]

The result now follows from the concentration (94) and the bound (98).

\[\square\]

### D.1 Metric learning: Proof of Lemma 5.1

Lemma 5.1 is simply a consequence of Proposition 11. Below we use notation \( C, C_1, C_2, \ldots \) to denote constants that depend only on \( M, M_X, \mu, p \). Throughout the section, we use the notation \( Z = (X, Y) \) to denote the data. We use \( Z, Z' \) to denote independent copies.

- We first prove the concentration of the objective value. We show that there exists a constant \( C > 0 \) such that for any \( \epsilon > 0 \), with probability at least \( 1 - e^{-n \epsilon^2} \):
  \[
  \sup_{\beta \in \mathcal{Z}} |F_{\text{ML}}(\beta; Q) - F_{\text{ML}}(\beta; Q_n)| \leq C \cdot \left( \frac{1}{\sqrt{n}} + \epsilon \right). \tag{99}
  \]
  Note that \( F_{\text{ML}}(\beta; Q) = \mathbb{E}[U_\beta(Z, Z')] \) where \( U_\beta(z, z') = yy' h(||x - x'||_{1,\beta}) \). As the function \( h \) is completely monotone, we know that the function \( h \) is uniformly bounded and Lipschitz on \( \mathbb{R}_+ \). As a consequence, the function \( \beta \mapsto U_\beta \) is bounded by \( C_1 \) and Lipschitz on the box constraint set \( \mathcal{Z} \) with the Lipschitz constant at most \( C_2 \). Now the concentration result in Eq. (99) simply follows from Proposition 11.

- We next prove the concentration of the gradient. We show that there exists a constant \( C > 0 \) such that for any \( \epsilon > 0 \), for any \( j \in [p] \), with probability at least \( 1 - e^{-n \epsilon^2} \):
  \[
  \sup_{\beta \in \mathcal{Z}} \left| \partial_{\beta_j} F_{\text{ML}}(\beta; Q) - \partial_{\beta_j} F_{\text{ML}}(\beta; Q_n) \right| \leq C \cdot \left( \frac{1}{\sqrt{n}} + \epsilon \right). \tag{100}
  \]
  Note that \( \partial_{\beta_j} F_{\text{ML}}(\beta; Q) = \mathbb{E}[U_\beta(Z, Z')] \) where \( U_\beta(z, z') = yy' h(||x - x'||_{1,\beta}) |x_j - x'_{j}| \). Similar to before, it’s easy to show that the function \( \beta \mapsto U_\beta \) is bounded by \( C_3 \) and Lipschitz on the box constraint set \( \mathcal{Z} \) with the Lipschitz constant at most \( C_4 \). Now the concentration result in Eq. (100) simply follows from Proposition 11.

Lemma 5.1 now follows from the concentration results in Eq. (99) and (100).
D.2 Kernel ridge regression: Proof of Lemma 5.3

Notation. Let \( \hat{f}_{\beta,\lambda} \) and \( f_{\beta,\lambda} \) denote the minimizer of the empirical and population kernel ridge regression. Mathematically, they are defined by the following equations:

\[
\hat{f}_{\beta,\lambda} = \arg\min_{f \in \mathcal{H}} \frac{1}{2} \mathbb{E}_{Q_n}[(Y - f(\beta^{1/q} \circ X))^2] + \frac{\lambda}{2} \|f\|_\mathcal{H}^2.
\]

\[
f_{\beta,\lambda} = \arg\min_{f \in \mathcal{H}} \frac{1}{2} \mathbb{E}_Q[(Y - f(\beta^{1/q} \circ X))^2] + \frac{\lambda}{2} \|f\|_\mathcal{H}^2.
\]

Let \( \tilde{\beta}(x, y) = y - \hat{f}_{\beta,\lambda}(\beta^{1/q} \circ x; y) \) and \( z_{\beta}(x, y) = y - f_{\beta,\lambda}(\beta^{1/q} \circ x; y) \). We use the notation \( Z = (X, Y) \) to denote the data. We use \( Z, Z' \) to denote independent copies.

Throughout the section, we use notation \( C, C_1, C_2, \ldots \), to denote constants that depend only on \( M, M_X, M_Y, \mu, p \). In particular, these constants do not depend on \( n, \lambda \).

Main Proof. Lemma 5.3 basically follows from Proposition 11.

- We first prove the concentration of the objective value. We show that there exists a constant \( C > 0 \) such that for any \( \epsilon > 0 \), with probability at least \( 1 - e^{-nc^2} \):

\[
\sup_{\beta \in \mathcal{Z}} \left| F_{\lambda}^{\text{KRR}}(\beta; Q) - F_{\lambda}^{\text{KRR}}(\beta; Q_n) \right| \leq \frac{C}{\lambda^{3/2}} \cdot \left( \frac{1}{\sqrt{n}} + \epsilon \right), \tag{101}
\]

According to Lemma A.5, we have the representation of the objective value:

\[
F_{\lambda}^{\text{KRR}}(\beta; Q) = \frac{1}{2} \mathbb{E}_Q[z_{\beta}(X; Y)Y] \quad \text{and} \quad F_{\lambda}^{\text{KRR}}(\beta; Q_n) = \frac{1}{2} \mathbb{E}_{Q_n}[\tilde{z}_{\beta}(X; Y)Y].
\]

To facilitate the proof, it’s natural to introduce the auxiliary quantity \( \overline{F}_{\lambda}^{\text{KRR}}(\beta) = \frac{1}{2} \mathbb{E}_{Q_n}[z_{\beta}(X; Y)Y] \). Below we show the existence of constants \( C_1, C_2 > 0 \) such that for any \( \epsilon > 0 \), the following holds with probability at least \( 1 - e^{-nc^2} \):

\[
\sup_{\beta \in \mathcal{Z}} \left| F_{\lambda}^{\text{KRR}}(\beta; Q) - \overline{F}_{\lambda}^{\text{KRR}}(\beta) \right| \leq \frac{C_1}{\lambda^{3/2}} \cdot \left( \frac{1}{\sqrt{n}} + \epsilon \right), \tag{102}
\]

\[
\sup_{\beta \in \mathcal{Z}} \left| F_{\lambda}^{\text{KRR}}(\beta; Q_n) - \overline{F}_{\lambda}^{\text{KRR}}(\beta) \right| \leq \frac{C_2}{\lambda^{3/2}} \cdot \left( \frac{1}{\sqrt{n}} + \epsilon \right). \tag{103}
\]

It’s clear that the desired concentration result (101) would follow immediately by the triangle inequality. It remains to prove the high probability bound (102) and (103).

The concentration (102) follows from a straightforward application of Proposition 11. Indeed, \( F_{\lambda}^{\text{KRR}}(\beta; Q) = \mathbb{E}_Q[U_{\beta}(Z, Z')] \) and \( \overline{F}_{\lambda}^{\text{KRR}}(\beta) = \mathbb{E}_{Q_n}[U_{\beta}(Z, Z')] \) where \( U_{\beta}(z, z') = \frac{1}{2}(y_{z_{\beta}(x; y)} + y'_{z_{\beta}(x'; y'))} \). Note the function \( \beta \mapsto U_{\beta}(z, z') \) is bounded by \( C_3/\lambda^{1/2} \) and is Lipschitz on the box constraint \( \mathcal{Z} \) with the Lipschitz constant at most \( C_4/\lambda^{3/2} \) when \( z, z' \in \text{supp}(Q) \), thanks to Lemma D.2 and the assumption that \( \text{supp}(Q) \) is compact. The concentration result thus follows.

The high probability bound in Eq. (103) is straightforward from Lemma D.1 and the Cauchy-Schwartz inequality (recall that \( |Y| \leq C_5 \) almost surely by assumption).
• Next we prove the concentration of the gradient. We show that there exists a constant $C > 0$ such that for any $\epsilon > 0$, for any $j \in [p]$, with probability at least $1 - e^{-n\epsilon^2}$:

$$\sup_{\beta \in Z} \left| \partial_{\beta_j} F_{\text{ML}}(\beta; Q) - \partial_{\beta_j} F_{\text{ML}}(\beta; Q_n) \right| \leq \frac{C}{\lambda^3} \cdot \left( \frac{1}{\sqrt{n}} + \epsilon \right).$$

(104)

According to Lemma A.6, we have the representation of the objective value:

$$\partial_{\beta_j} F_{\text{KRR}}(\beta; Q) = -\frac{1}{\lambda} \mathbf{E}_{Q_n} \left[ z_\beta(X; Y)z_\beta(X'; Y')h(\|X - X'\|_q^q)\right],$$

$$\partial_{\beta_j} F_{\text{KRR}}(\beta; Q_n) = -\frac{1}{\lambda} \mathbf{E}_{Q_n} \left[ \tilde{z}_\beta(X; Y)\tilde{z}_\beta(X'; Y')h(\|X - X'\|_q^q)\right].$$

To facilitate the proof, it’s natural to introduce the auxiliary quantity

$$\overline{F_{\text{KRR}}}(\beta) = -\frac{1}{\lambda} \mathbf{E}_{Q_n} \left[ z_\beta(X; Y)z_\beta(X'; Y')h(\|X - X'\|_q^q)\right].$$

Below we show the existence of constants $C_1, C_2 > 0$ such that for any $\epsilon > 0$, the following holds with probability at least $1 - e^{-n\epsilon^2}$:

$$\sup_{\beta \in Z} \left| F_{\text{KRR}}(\beta; Q) - \overline{F_{\text{KRR}}}(\beta) \right| \leq \frac{C_1}{\lambda^3} \cdot \left( \frac{1}{\sqrt{n}} + \epsilon \right)$$

(105)

$$\sup_{\beta \in Z} \left| F_{\text{KRR}}(\beta; Q_n) - \overline{F_{\text{KRR}}}(\beta) \right| \leq \frac{C_2}{\lambda^3} \cdot \left( \frac{1}{\sqrt{n}} + \epsilon \right).$$

(106)

It’s clear that the desired concentration result (104) would follow immediately by the triangle inequality. It remains to prove the high probability bound (105) and (106).

The concentration (105) follows from a straightforward application of Proposition 11. Indeed, $F_{\text{KRR}}(\beta; Q) = \mathbf{E}_{Q}[U_\beta(Z, Z')]$ and $\overline{F_{\text{KRR}}}(\beta) = \mathbf{E}_{Q_n}[U_\beta(Z, Z')]$ where the function $U_\beta(z, z') = -\frac{1}{2} z_\beta(x; y)z_\beta(x'; y')h(\|x - x'\|^q)$. Note the function $\beta \mapsto U_\beta(z, z')$ is bounded by $C_3/\lambda^3$ and is Lipschitz on the box constraint $Z$ with the Lipschitz constant at most $C_3/\lambda^3$ when $z, z' \in \text{supp}(Q)$, thanks to Lemma D.2 and the assumption that supp$(Q)$ is compact. The concentration result thus follows.

The proof of high probability bound in Eq. (106) is straightforward. Indeed, (i) $|Y| \leq C_5$ almost surely by assumption and (ii) $\sup_x |h'(x)| \leq |h'(0)|$. Hence, the bound follows from Lemma D.1 and Cauchy-Schwartz inequality.

Lemma 5.1 now follows from the concentration results in Eq. (101) and (104).

### D.3 Technical lemma for kernel ridge regression

**Lemma D.1** (Concentration of $\tilde{z}_{\beta; \lambda}$ to $z_{\beta; \lambda}$). There exists some constant $C > 0$ such that the following holds: for any $\epsilon > 0$, with probability at least $1 - e^{-n\epsilon^2}$

$$\sup_{\beta \in Z} \left( \mathbf{E}_{Q_n}[(\tilde{z}_\beta(X, Y) - z_\beta(X, Y))^2] \right)^{1/2} \leq \frac{C}{\lambda} \cdot \left( \frac{1}{\sqrt{n}} + \epsilon \right),$$

where the constant $C > 0$ depends only on $M, M_X, M_Y, \mu, p$ and not on $n, \lambda$.  

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Lemma D.2 (Properties of the mapping $\beta \mapsto f_{\beta;\lambda}$). The mapping $\beta \mapsto f_{\beta;\lambda}$ satisfies:

- **Uniform Boundedness**: $\|f_{\beta;\lambda}\|_\infty \leq \frac{C}{\lambda^{1/2}}$ for all $\beta \in \mathbb{Z}$.

- **Hölder Continuity**: $\|f_{\beta;\lambda} - f_{\beta';\lambda}\|_\infty \leq \frac{C}{\lambda^{1/2}} \|\beta - \beta'\|_1^{1/2}$ for all $\beta, \beta' \in \mathbb{Z}$, where the constant $C > 0$ depends only on $M, M_X, M_Y, \mu, p$ and not on $n, \lambda$.

D.4 Proof of Lemma D.1 and Lemma D.2

D.4.1 Preliminaries I

We introduce a new representation of $f_{\beta;\lambda}$ and $\hat{f}_{\beta;\lambda}$ using the functional analytic tools in the literature [Baker 1973, Ruan et al. 2021]. These tools are particularly useful to derive perturbation bounds, and in particular to derive Lemma D.1 and Lemma D.2. Recall $k(x, x') = h(||x - x'||^q_q)$.

**Definition D.1.** We define the population and empirical covariance operator $\Sigma_\beta : \mathcal{H} \mapsto \mathcal{H}$, $\hat{\Sigma}_\beta : \mathcal{H} \to \mathcal{H}$ as the bounded linear operators that satisfy for any $f \in \mathcal{H}$

$$
\Sigma_\beta f = \mathbb{E}_{Q}[k((\beta^{1/q} \circ X, \cdot)f((\beta^{1/q} \circ X))],
$$

$$
\hat{\Sigma}_\beta f = \mathbb{E}_{Q_n}[k((\beta^{1/q} \circ X, \cdot)f((\beta^{1/q} \circ X))].
$$

We define the population and empirical covariance function $h_\beta \in \mathcal{H}$, $\hat{h}_\beta \in \mathcal{H}$ by

$$
h_\beta = \mathbb{E}_Q[Yk(\beta^{1/q} \circ X, \cdot)] \quad \text{and} \quad \hat{h}_\beta = \mathbb{E}_{Q_n}[Yk(\beta^{1/q} \circ X, \cdot)].
$$

**Lemma D.3** (Representation of the solution $f_{\beta;\lambda}$ and $\hat{f}_{\beta;\lambda}$ in terms of the covariance operators and covariance functions). We have the following representation

$$
f_{\beta;\lambda} = (\Sigma_\beta + \lambda I)^{-1}h_\beta \quad \text{and} \quad \hat{f}_{\beta;\lambda} = (\hat{\Sigma}_\beta + \lambda I)^{-1}\hat{h}_\beta.
$$

D.4.2 Preliminaries II

We introduce a high probability concentration result that underlies the proof of Lemma D.2. The proof of Lemma D.4 is given in Section D.4.5.

**Lemma D.4** (Concentration of the covariance operators and covariance functions). There exists some constant $C > 0$ such that the following holds: for any $\epsilon > 0$, with probability at least $1 - e^{-n\epsilon^2}$, the following bound holds:

$$
\sup_{\beta \in \mathbb{Z}} \|h_\beta - \hat{h}_\beta\|_{\mathcal{H}} \leq C \cdot \left(\frac{1}{\sqrt{n}} + \epsilon\right) \quad \text{and} \quad \sup_{\beta \in \mathbb{Z}} \|\Sigma_\beta - \hat{\Sigma}_\beta\|_{\text{op}} \leq C \cdot \left(\frac{1}{\sqrt{n}} + \epsilon\right),
$$

where the constant $C > 0$ depends only on $M, M_X, M_Y, \mu, p$ and not on $n, \lambda$.

**Proof** The proof is based on the technique that underlies the proof of Lemma E.3 in Ruan et al. (2021), albeit there is slight change in the evaluation of the metric entropy integral. For completeness, we provide the proof in Section D.4.5.
D.4.3 Proof of Lemma D.1

Our starting point is the following identity:

\[
\left(\mathbb{E}_{Q_n}(\tilde{z}_\beta(X,Y) - z_\beta(X,Y))^2\right)^{1/2} = \|\hat{\Sigma}_\beta^{1/2}(f_{\beta;\lambda} - \hat{f}_{\beta;\lambda})\|_\mathcal{H}. \tag{107}
\]

Indeed, note that (i) \( \tilde{z}_\beta(x,y) - z_\beta(x,y) = (f_{\beta;\lambda} - \hat{f}_{\beta;\lambda})(\beta^{1/q} \circ x) \) and (ii) \( \mathbb{E}_{Q_n}[g^2(\beta^{1/q} \circ X)]^{1/2} = \|\hat{\Sigma}_\beta^{1/2}g\|_\mathcal{H} \) holds for all \( g \in \mathcal{H} \). Below we shall prove the deterministic bound:

\[
\|\hat{\Sigma}_\beta^{1/2}(f_{\beta;\lambda} - \hat{f}_{\beta;\lambda})\|_\mathcal{H} \leq \frac{1}{\lambda} M_Y \cdot \left(\|\Sigma_\beta - \hat{\Sigma}_\beta\|_{op} + \|h_\beta - \hat{h}_\beta\|_\mathcal{H}\right). \tag{108}
\]

Now Lemma D.1 follows immediately from Lemma D.4.

It remains to prove Eq. (108). The proof is based on simple algebra. The starting point is the following error decomposition: \( \hat{\Sigma}_\beta^{1/2}(f_{\beta;\lambda} - \hat{f}_{\beta;\lambda}) = \mathcal{E}_1 + \mathcal{E}_2 \) where

\[
\mathcal{E}_1 = \hat{\Sigma}_\beta^{1/2}(\Sigma_\beta + \lambda I)^{-1} - (\hat{\Sigma}_\beta + \lambda I)^{-1}\hat{h}_\beta, \quad \mathcal{E}_2 = \hat{\Sigma}_\beta^{1/2}(\Sigma_\beta + \lambda I)^{-1}(h_\beta - \hat{h}_\beta).
\]

As a result, \( \|\hat{\Sigma}_\beta^{1/2}(f_{\beta;\lambda} - \hat{f}_{\beta;\lambda})\|_\mathcal{H} \leq \|\mathcal{E}_1\|_\mathcal{H} + \|\mathcal{E}_2\|_\mathcal{H} \). Below we bound \( \|\mathcal{E}_1\|_\mathcal{H} \) and \( \|\mathcal{E}_2\|_\mathcal{H} \).

**Bound on \( \|\mathcal{E}_1\|_\mathcal{H} \)** Simple algebraic manipulation yields the following identity:

\[
\mathcal{E}_1 = \left(\hat{\Sigma}_\beta^{1/2}(\hat{\Sigma}_\beta + \lambda I)^{-1/2}\right) \cdot \left(I - (\hat{\Sigma}_\beta + \lambda I)^{-1/2}(\Sigma_\beta + \lambda I)^{-1}(\hat{\Sigma}_\beta + \lambda I)^{1/2}\right) \cdot \left((\hat{\Sigma}_\beta + \lambda I)^{-1/2}\hat{h}_\beta\right).
\]

Now we bound the above three terms on the right-hand side.

- \( \Sigma_\beta \) is a positive operator. Hence, \( \|\hat{\Sigma}_\beta^{1/2}(\Sigma_\beta + \lambda I)^{-1/2}\|_{op} \leq 1 \).

- We use the following fundamental fact in functional analysis. For any linear operator \( A : \mathcal{H} \to \mathcal{H} \), denoting \( A^* \) to its adjoint operator, then \( I - A^*A \) has the same spectrum as \( I - AA^* \). Applying this to the operator \( A = (\Sigma_\beta + \lambda I)^{1/2}(\Sigma_\beta + \lambda I)^{-1/2} \), we obtain

\[
\|I - (\hat{\Sigma}_\beta + \lambda I)^{-1/2}(\Sigma_\beta + \lambda I)^{-1}(\hat{\Sigma}_\beta + \lambda I)^{1/2}\|_{op} \leq \frac{1}{\lambda} \|\Sigma_\beta - \hat{\Sigma}_\beta\|_{op}. \tag{109}
\]

- We have the bound \( \|((\hat{\Sigma}_\beta + \lambda I)^{-1/2}\hat{h}_\beta\|_\mathcal{H} \leq M_Y \). Indeed, the bound appears in the proof of Proposition 10 in [Ruan et al. (2021)].

As a summary, we have proven that \( \|\mathcal{E}_1\|_\mathcal{H} \leq \frac{1}{\lambda} M_Y \cdot \|\Sigma_\beta - \hat{\Sigma}_\beta\|_{op} \).

**Bound on \( \|\mathcal{E}_2\|_\mathcal{H} \)** Recall \( \mathcal{E}_2 = \hat{\Sigma}_\beta^{1/2} \cdot (\Sigma_\beta + \lambda I)^{-1} \cdot (h_\beta - \hat{h}_\beta) \). Note the following bounds.

- \( \|\hat{\Sigma}_\beta^{1/2}\|_{op} \leq \|h(0)\|^{1/2} \). This is true since by Lemma A.3, any function \( g \in \mathcal{H} \) satisfies

\[
\|\hat{\Sigma}_\beta^{1/2}g\|_\mathcal{H} = \mathbb{E}_{Q_n}[g^2(X)]^{1/2} \leq \|g\|_\infty \leq \|h(0)\|^{1/2} \cdot \|g\|_\mathcal{H}.
\]

- \( \|\Sigma_\beta + \lambda I\|_{op} \leq \frac{1}{\lambda} \) since \( \Sigma_\beta \) is a positive operator.

As a result, this proves that \( \|\mathcal{E}_2\|_\mathcal{H} \leq \frac{1}{\lambda} \cdot \|h(0)\|^{1/2} \cdot \|h_\beta - \hat{h}_\beta\|_\mathcal{H} \).
Summary  As a result, we have shown Eq. (108). Lemma D.1 follows from Lemma D.4.

D.4.4 Proof of Lemma D.2

• The Hölder’s continuity follows from the basic algebra. By Lemma A.3, it suffices to prove for some constant $C > 0$ depending only on $M, M_X, M_Y, \mu, p$ and not on $n, \lambda$.

$$\|f_{\beta;\lambda} - f_{\beta';\lambda}\|_H \leq \frac{C}{\lambda^{3/2}} \|\beta - \beta'\|_1^{1/q}.$$ Now we bound $\|f_{\beta;\lambda} - f_{\beta';\lambda}\|_H$. We start from the representation due to Lemma D.2:

$$f_{\beta;\lambda} = (\Sigma_\beta + \lambda I)^{-1}h_\beta \text{ and } f_{\beta';\lambda} = (\Sigma_\beta' + \lambda I)^{-1}h_\beta'$$

Simple algebraic manipulation gives

$$f_{\beta;\lambda} - f_{\beta';\lambda} = (\Sigma_\beta + \lambda I)^{-1}(\Sigma_\beta' - \Sigma_\beta)\Sigma_\beta + \lambda I)^{-1}h_\beta + (\Sigma_\beta' + \lambda I)^{-1}(h_\beta - h_\beta').$$

Note the following bounds: (i) $\|(\Sigma_\beta + \lambda I)^{-1/2}h_\beta\|_H \leq M_Y$—this basic bound appears in the proof of Proposition 10 in Ruan et al. (2021) (ii) $\|\Sigma_\beta + \lambda I\|^{1/2} \leq \frac{1}{\lambda}$. As a consequence, we immediately obtain the following bound:

$$\|f_{\beta;\lambda} - f_{\beta';\lambda}\|_H \leq 1 \cdot \left( M_Y \cdot \|\Sigma_\beta - \Sigma_\beta'\|_\text{op} + \|h_\beta - h_\beta'\|_H \right)$$

Now it remains to bound $\|\Sigma_\beta - \Sigma_\beta'\|_\text{op}$ and $\|h_\beta - h_\beta'\|_H$. We do some simple algebra. Let $(X,Y), (X',Y')$ be independent copies drawn from $Q$. Following the proof of Proposition 11 in Ruan et al. (2021), we have the following identity:

$$h_\beta - h_\beta' = \mathbb{E}[(k_{\beta_1,\beta_2}(x, x') + k_{\beta'_1,\beta'_2}(X, X') - 2k_{\beta,\beta'}(X, X')YY')]$$

where $k_{\beta_1,\beta_2}(x, x') = h((|\beta_1^{1/q} \circ x - \beta_2^{1/q} \circ x'|^q)^{1/q})$. Additionally, we have the inequality:

$$\|\Sigma_\beta - \Sigma_\beta'\|_\text{op}^2 \leq \mathbb{E}[(k_{\beta_1,\beta_2}(X, X') + k_{\beta'_1,\beta'_2}(X, X') - 2k_{\beta,\beta'}(X, X')YY')]$$

With some diligent algebraic manipulations and basic analytic tools (e.g., Taylor’s intermediate theorem), the above two equations (110) and (111) immediately yield

$$\|h_\beta - h_\beta'\|_H \leq C \|\beta - \beta'\|_1^{1/2q} \text{ and } \|\Sigma_\beta - \Sigma_\beta'\|_\text{op} \leq C \|\beta - \beta'\|_1^{1/2q}$$

where the constant $C$ depends only on $M, M_X, M_Y, \mu, p$ and not on $n, \lambda$. 

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D.4.5 Proof of Lemma D.4

The proof here largely follows the proof of Lemma E.3 in [Ruan et al. (2021)]. Only slight modification is needed. Below we only prove the concentration for the covariance function (i.e., \( \hat{h}_\beta \approx h_\beta \) uniformly over \( \beta \in \mathcal{Z} \)), as the proof for the covariance operator (i.e., \( \hat{\Sigma}_\beta \approx \Sigma_\beta \)) is totally analogous. Below we use \( C, C_1, C_2, \ldots \), to denote constants that depend only on \( M, M_X, M_Y, \mu, p \) and not on \( n, \lambda \).

**Step 1: Symmetrization and Reduction** Let \( \epsilon \) denote independent Rademacher random variables. Let \( \hat{h}_\beta(\epsilon) = \mathbb{E}_{Q_n}[k(\beta^{1/q} \odot X, \cdot) Y] \). The standard symmetrization argument gives the following bound that holds for any convex and increasing mapping \( \Phi : \mathbb{R}_+ \to \mathbb{R}_+ \):

\[
\mathbb{E} \left[ \Phi \left( \sup_{\beta \in \mathcal{Z}} \| h_\beta - \hat{h}_\beta \|_{\mathcal{H}} \right) \right] \leq \mathbb{E} \left[ \Phi \left( 2 \cdot \sup_{\beta \in \mathcal{Z}} \| \hat{h}_\beta(\epsilon) \|_{\mathcal{H}} \right) \right]
\]

A classical reduction argument due to Panchenko (Lemma I.1 in [Ruan et al. (2021)]) implies that it suffices to derive an exponential tail bound on \( \sup_{\beta \in \mathcal{Z}} \| \hat{h}_\beta(\epsilon) \|_{\mathcal{H}} \).

**Step 2: Evaluation and Simplification** The reproducing property of \( k \) shows that

\[
\| \hat{h}_\beta(\epsilon) \|^2_{\mathcal{H}} = \mathbb{E}_{Q_n} \left[ \epsilon^\top h(\|X - X'\|^{q}_{\mathcal{Q},\beta}) Y Y' \right],
\]

where \((X, Y), (X', Y') \) above are independently sampled from \( Q_n \). Write \( W_\beta = \| \hat{h}_\beta(\epsilon) \|^2_{\mathcal{H}} \).

**Step 3: Centering** Write \( \overline{W}_\beta = W_\beta - \mathbb{E}[W_\beta] \). Let \( W = \sup_{\beta \in \mathcal{Z}} \overline{W}_\beta \) be the supremum of the centered process \( \overline{W}_\beta \). Since \( |\mathbb{E}[W_\beta]| \leq C/n \) for all \( \beta \) where \( C = |h(0)|^{1/2} M_Y \), we obtain the bound \( \sup_\beta W_\beta \leq W + C/n \). Below we control \( W \) by first control individual \( \overline{W}_\beta \).

**Step 4: Control \( \overline{W}_\beta \)** We use Hanson-Wright’s inequality to establish the sub-exponential property of the difference \( \overline{W}_\beta - \overline{W}_{\beta'} \). Clearly \( \epsilon Y \) is sub-gaussian. Now, let \( \{ (\mathcal{E}(i), X(i), Y(i)) \}_{i=1}^n \) be the i.i.d data. Introduce the matrix \( A_\beta \in \mathbb{R}^{n \times n} \) where its \((i, j)\)-th entry is defined by

\[
(A_\beta)_{i,j} = h(\|X^{(i)} - X^{(j)}\|^{q}_{\mathcal{Q},\beta}) - \mathbb{E}[h(\|X^{(i)} - X^{(j)}\|^{q}_{\mathcal{Q},\beta})].
\]

Let \( \Delta_{\beta, \beta'} \) be the matrix with \( \Delta_{\beta, \beta'} = A_\beta - A_{\beta'} \). Hanson-Wright’s inequality yields that

\[
\mathbb{P} \left( |\overline{W}_\beta - \overline{W}_{\beta'}| \geq t \mid X \right) \leq 2 \exp \left( -C_1 \cdot \min \left\{ -n^2 t/ \| \Delta_{\beta, \beta'} \|_{\mathcal{F}}^2, n^4 t^2/ \| \Delta_{\beta, \beta'} \|_{\mathcal{F}}^2 \right\} \right).
\]

Note that \( \max_{i,j} |\Delta_{\beta, \beta'}| \leq C_2 \cdot \| \beta - \beta' \|_{\infty} \) in virtue of the Lipschitzness of the kernel \( k \). Hence, we obtain \( \| \Delta_{\beta, \beta'} \|_{\mathcal{F}} \leq n \cdot C_2 \| \beta - \beta' \|_{\infty} \) and \( \| \Delta_{\beta, \beta'} \|_{\mathcal{F}} \leq n \cdot C_2 \| \beta - \beta' \|_{\infty} \). Consequently, we obtain that the increment \( |\overline{W}_\beta - \overline{W}_{\beta'}| \) is sub-exponential with

\[
\mathbb{P} \left( |\overline{W}_\beta - \overline{W}_{\beta'}| \geq t \right) \leq 2 \exp \left( -C_3 \cdot \min \left\{ -nt/ \| \beta - \beta' \|_{\infty}, n^2 t^2/ \| \beta - \beta' \|_{\infty}^2 \right\} \right).
\]
Step 5: Control $W$ via Chaining  The previous step shows that the process $\beta \rightarrow W_{\beta}$ has increments that are sub-exponential with parameter on the scale of $\|\beta - \beta'\|_\infty / n$. The chaining argument for the sub-exponential process (see Theorem 8 in [Ruan et al. (2021)]) implies that the following bound holds with probability at least $1 - e^{-nt}$:

$$W \leq C_4 \cdot \left( \frac{1}{n} \cdot \int_0^\infty \log N(Z, \|\cdot\|_\infty, \epsilon)de + t \right). \quad (112)$$

where $N(Z, \|\cdot\|_\infty, \epsilon)$ is the covering number of the set $Z$ using the $\|\cdot\|_\infty$-ball of radius $\epsilon$. As $\log N(Z, \|\cdot\|, \epsilon) = 0$ for $\epsilon > M$ and $\log N(Z, \|\cdot\|, \epsilon) \leq p \log(3M/\epsilon)$ for $\epsilon \leq M$, we obtain

$$\int_0^\infty \log N(Z, \|\cdot\|_\infty, \epsilon)de \leq 3Mp \cdot \int_0^{1/3} \log(1/\epsilon)de \leq C_5. \quad (113)$$

Consequently, we obtain that $W \leq C_5 \cdot (1/n + t)$ holds with probability at least $1 - e^{-nt}$.

Step 6: Finalizing Argument  Combine the results in Step 3 and Step 5. The following bound holds with probability at least $1 - e^{-nt}$ for any $t > 0$:

$$\sup_{\beta \in B_M} \|\hat{h}_\beta(\epsilon)\|_H = \sup_{\beta} W_{\beta}^{1/2} \leq C_7 \cdot \left( \frac{1}{\sqrt{n}} + \sqrt{t} \right).$$

As discussed in Step 1, Panchenko’s argument translates it to the desired high probability bound, i.e., $\sup_{\beta \in B_M} \|\hat{h}_\beta - h_\beta\|_H \leq C_7 \cdot \left( \frac{1}{\sqrt{n}} + \epsilon \right)$ with probability at least $1 - e^{-nc^2}$.

E  Statistical Consequence

E.1 Metric learning: Proof of Proposition 8

The main building block of the proof is Lemma [E.1] whose proof is given in Section [E.1.1]. Although independently stated, Lemma [E.1] is in fact a consequence of Theorem [1A]

**Lemma E.1.** Assume Assumptions [1] and [2]. Fix $\beta(0) \in Z$ of full support: $\text{supp}(\beta(0)) = [p]$. There exist constants $c, C, \epsilon_0 > 0$ such that the following holds. For any subset $A \subseteq [p]$, consider the following empirical minimization problem

$$\min_{\beta} F_{\text{ML}}(\beta; Q_n^A) \quad \text{subject to} \quad \beta \geq 0, \|\beta\|_\infty \leq M.$$

Let $\hat{\beta}$ be the stationary point found by the projected gradient flow initialized at $\beta(0)$. Then the following property holds with probability at least $1 - e^{-nc^2}$ if $\epsilon \geq C/\sqrt{n}$:

- If $E[Y|X] = E[Y|X_A]$, then $F_{\text{ML}}(\hat{\beta}; Q_n^A) > -\epsilon$

- Otherwise, then $\text{supp}(\hat{\beta}) \subseteq S$, $\text{supp}(\hat{\beta}) \setminus A \neq \emptyset$, $F_{\text{ML}}(\hat{\beta}; Q_n^A) < -\epsilon$ if $\epsilon_0 \geq \epsilon$,

where the constants $c, C, \epsilon_0$ are independent of the sample size $n$.  

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Now we are ready to prove Proposition 8. We take the same constants $c, \epsilon_0$ as described in Lemma E.1. We use $\Omega_n(A)$ to denote the event on which the property stated in Lemma E.1 holds. We take $\Omega_n \equiv \cap_{A \subseteq \mathbb{S}} \Omega_n(A)$ which we simply call it the “good event”. On the event $\Omega_n$, with a simple induction argument, one can show that Algorithm 1 must return a set $\hat{S}$ which simultaneously satisfies $\hat{S} \subseteq S$ and $\mathbb{E}[Y|X] = \mathbb{E}[Y|X_S]$. Clearly, this proves Proposition 8 as the good event $\Omega_n$ happens with probability at least $1 - 2^{|\mathbb{S}|}e^{-cn}$ by the union bound.

### E.1.1 Proof of Lemma E.1

The proof is similar to that of Theorem 1A. Consider the following “good” event $\Omega^A_n(\epsilon)$:

$$|F_{\text{ML}}(\beta; Q^n_A) - F_{\text{ML}}(\beta; Q^A)| \leq \epsilon, \quad \|\nabla F_{\text{ML}}(\beta; Q^n_A) - \nabla F_{\text{ML}}(\beta; Q^A)\|_{\infty} \leq \epsilon$$

for all $\beta \in \mathbb{Z}$.

Notice that the event $\Omega^A_n(\epsilon)$ is defined in a similar way to that of $\Omega_n(\epsilon)$ (cf. Eq. (37) in the main text). A similar proof to Lemma 5.1 implies that the event $\Omega^A_n(\epsilon)$ happens with high probability at least $1 - e^{-c\epsilon^2}$ for any $\epsilon \geq C/\sqrt{n}$.

We are now ready to prove Lemma E.1.

- Assume $\mathbb{E}[Y|X] = \mathbb{E}[Y|X_A]$. According to Proposition 3 and Proposition 4 in Liu and Ruan (2020), $X \perp Y$ under the reweighting distribution $Q^A$, and $F_{\text{ML}}(\beta; Q^A) \equiv 0$. As a consequence, we have $F_{\text{ML}}(\beta; Q^n_A) > -\epsilon$ for all $\beta \in \mathbb{Z}$ on the event $\Omega^A_n(\epsilon)$.

- Assume otherwise. Then $X^A \not\perp Y$ under $Q^A$. Furthermore, if we denote $S^A$ to be the signal set under $Q^A$ according to Definition 3.1, then $S^A \subseteq S$ and $S^A \setminus A \neq \emptyset$ according to Proposition 3 in Liu and Ruan (2020). As a result, we have $|F_{\text{ML}}(\beta(0); Q^A)| > 0$ since $F_{\text{ML}}$ is an independence measure and $\beta(0)$ is of full support. Let $\epsilon_0 = |F_{\text{ML}}(\beta(0); Q^A)|/4$. An almost identical proof of Theorem 1A gives that $\text{supp}(\beta(0)) \subseteq S$, $\text{supp}(\hat{\beta}) \setminus A \neq \emptyset$ and $F_{\text{ML}}(\hat{\beta}; Q^n_A) < -\epsilon$ on $\Omega^A_n(\epsilon)$ for all $\epsilon \leq \epsilon_0/2$.

### E.2 Kernel ridge regression: Proof of Proposition 9

The main building block of the proof is Lemma E.2 whose proof is given in Section E.2.1. Although independently stated, Lemma E.2 is in fact a consequence of Theorem 1B.

**Lemma E.2.** Assume Assumptions 1B. Let $q = 1$. There exist constants $c, C, \epsilon_0, \lambda_0 > 0$ such that the following holds. For any subset $A \subseteq [p]$, consider the empirical minimization

$$\min_{\beta} F_{\text{KRR}}(\beta; Q_n) \quad \text{subject to} \quad \beta \geq 0, \quad \beta_A = M1_A, \quad \|\beta\|_{\infty} \leq M.$$

Let $\hat{\beta}$ be the stationary point found by the projected gradient flow initialized at $\beta(0) = \beta^{(0);A}$ (which is defined in the statement of Proposition 9). For any $\lambda \leq \lambda_0$, $\epsilon \geq C/(\sqrt{n}\lambda^3)$, there exists an event $\Omega_n \equiv \Omega_n(\epsilon)$ whose definition is independent of the subset $A$ and which happens with probability at least $1 - e^{-cn(\epsilon^2 + \lambda^2)\lambda^6}$ such that the following happens on $\Omega_n$:

- If $\mathbb{E}[Y|X] = \mathbb{E}[Y|X_A]$, then $F^\lambda_{\text{KRR}}(\beta^{*}; Q_n) - F^\lambda_{\text{KRR}}(\hat{\beta}; Q_n) < \epsilon$.  

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where the constants $c, C, \epsilon_0$ are independent of the sample size $n$.

Now we are ready to prove Proposition 9. We take the same constants $c, \epsilon_0$ as described in Lemma E.2. Fix the parameter $\epsilon_0 > 0$ from the statement of Proposition 9. We use $\Omega_n$ to denote the event described in Lemma E.2. On the event $\Omega_n$, with a simple induction argument, one can easily show that Algorithm 2 must return a set $\hat{S}$ which simultaneously satisfies $\hat{S} \subseteq S$ and $\mathbb{E}[|X|] = \mathbb{E}[|X_{\bar{S}}|]$. This proves Proposition 9 as the good event $\Omega_n$ happens with probability at least $1 - e^{-cn(\epsilon^2 + \lambda^2)\lambda_0}$.

### E.2.1 Proof of Lemma E.2

The proof is similar to that of Theorem 1B. Recall the event $\Omega_n(\epsilon)$ (cf. Eq. (45)):

$$
\| F^{\text{KRR}}(\beta; Q_n) - F^{\text{KRR}}(\beta; Q) \|_{\infty} \leq \epsilon \\
\| \nabla F^{\text{KRR}}(\beta; Q_n) - \nabla F^{\text{KRR}}(\beta; Q) \|_{\infty} \leq \epsilon
$$

Lemma 5.3 implies that the event $\Omega_n(\epsilon)$ happens with high probability at least $1 - e^{-cn(\epsilon^2 + \lambda^2)}$ for any $\epsilon \geq C/(\sqrt{n}\lambda^3)$.

Now is an opportune time to prove Lemma E.2. Below we fix $\epsilon > 0$.

- Assume $\mathbb{E}[|X|] = \mathbb{E}[|X_{\bar{S}}|]$. According to Proposition 3, there exists $\lambda_0 > 0$ such that for $\lambda \leq \lambda_0$: $F^{\text{KRR}}(\beta^*; \lambda; Q) < G + \epsilon/2$ where $G = \frac{1}{2}\text{Var}(\mathbb{E}_Q[|X|])$. It’s easy to show that $F^{\text{KRR}}(\beta; Q) > G$ for all $\beta \in \mathbb{Z}$ and $\lambda \geq 0$. Hence, this shows that $F^{\text{KRR}}(\beta^* A; Q) - F^{\text{KRR}}(\beta; Q) < \epsilon/2$ for all $\beta \in \mathbb{Z}$. By triangle inequality, this implies that $F^{\text{KRR}}(\beta^* A; Q) - F^{\text{KRR}}(\beta; Q) < \epsilon$ for all $\beta \in \mathbb{Z}$ on the event $\Omega_n(\epsilon/4)$.

- Assume otherwise. Then there exists a feature $X_i$ such that $\mathbb{E}[|X_{\bar{A}}|] \neq \mathbb{E}[|X_{\bar{A}\cup\{i\}}|]$. Proposition A.13 shows a lower bound on the gradient: $\partial_{\beta} F(\beta; Q) \geq c/\lambda$ at $\beta = \beta^* A = \beta^0 A$ where $c > 0$ is a constant independent of $n$ and $\lambda$. The rest of the proof then follows exactly the same logic as appeared in the proof of Theorem 1B. That means that, for some $\epsilon_0 > 0$, we must have on the event $\Omega_n(\epsilon_0\lambda)$, $\text{supp}(\tilde{\beta}) \subseteq S$, $\text{supp}(\hat{\beta}) \neq \emptyset$, $F^{\text{KRR}}(\beta^* A, Q_n) - F^{\text{KRR}}(\beta; Q_n) > \epsilon_0$.

### F Other Results

#### F.1 Extension: Relaxation of the independence assumption $X_S \perp X_{S^c}$

**Definition F.1.** The maximal correlation between two groups of random variables $W_1, W_2$ is defined by

$$
\vartheta(W_1, W_2) = \sup_{g_1, g_2} \frac{\text{Cov}(g_1(W_1), g_2(W_2))}{\sqrt{\text{Var}(g_1(W_1))\text{Var}(g_2(W_2))}}
$$

where the supremum is taken over all real-valued measurable functions such that $\text{Var}(g_1(W_1)) < \infty$ and $\text{Var}(g_2(W_2)) < \infty$. 


Theorem 1A’ is a viable extension of Theorem 1A. Basically, Theorem 1A allows weak dependence between the signal variables $X_S$ and the noise variables $X_{Sc}$ (while Theorem 1A requires exact independence between $X_S$ and $X_{Sc}$).

**Theorem 1A’.** Assume Assumptions 1 and 2. Assume the set of signals is not empty: $S \neq \emptyset$. Consider the trajectory $t \mapsto \beta(t)$ of the gradient flow with respect to the empirical metric learning objective $F_{\text{ML}}(\cdot; \mathbb{Q}_n)$. Choose the initialization to be of full support: $\text{supp}(\beta(0)) = [p]$. Then there exists $\vartheta_0 > 0$ such that the following holds. As long as $\vartheta(X_S, X_{Sc}) \leq \vartheta_0$, the following happens with probability at least $1 - e^{-c n}$:

$$\emptyset \neq \text{supp}(\beta(t)) \subseteq S \quad \text{holds for all } t \geq \tau,$$

where the constants $c, \tau > 0$ are independent of the sample size $n$.

**Proof** The proof of Theorem 1A’ follows the exact same route as that of Theorem 1A. Indeed, it suffices to show that the population objective $F_{\text{ML}}(\cdot; \mathbb{Q})$ is self-penalizing when there is the weak dependence $\vartheta(X_S, X_{Sc}) \leq \vartheta_0$ for some $\vartheta_0 > 0$. This is implied by the following Theorem 2’ which is a generalization of the gradient bound of Theorem 2 to the weak dependence setting.

**Theorem 2’.** Assume Assumptions 1 and 2. The following holds for all $\beta \geq 0$ and $j \notin S$:

$$\partial_\beta \vartheta_{\beta_j} F_{\text{ML}}(\beta; \mathbb{Q}) \geq c(\beta) \cdot |F_{\text{ML}}(\beta; \mathbb{Q})| - C \vartheta(X_S, X_{Sc}).$$

(114)

where $c(\beta) > 0$ is defined in Theorem 2 and $C > 0$ depends only on $M_\mu, M_X$.

**Proof** The big picture of the proof of Theorem 2 is identical to that of Theorem 2 (Section 4.5). We only need to do some minor tweaks. There are only two lines of derivations in the proof of Theorem 2 where we’ve used the independence assumption $X_S \perp X_{Sc}$, namely, equations (28) and (29). There we use the independence assumption $X_S \perp X_{Sc}$ to attain the identity $E[g_1(X_S)g_2(X_{Sc})] = E[g_1(X_S)]E[g_2(X_{Sc})]$ that holds for any real-valued functions $g_1, g_2$. More generally, without the independence assumption $X_S \perp X_{Sc}$, we instead attain a bound than an identity that holds for all functions $g_1, g_2$:

$$E[g_1(X_S)g_2(X_{Sc})] \in \left[ E[g_1(X_S)]E[g_2(X_{Sc})] \pm \vartheta(X_S, X_{Sc}) \sqrt{\text{Var}(g_1(X_S))\text{Var}(g_2(X_{Sc}))} \right],$$

where the notation $[a \pm b]$ means the interval $[a - b, a + b]$ for any $a \in \mathbb{R}, b \in \mathbb{R}_+$. Hence, the analogue of Eq. (28) in the more general setting is simply the following:

$$E_Q \left[ YY' e^{-t\|X - X'\|_{q, \beta}^q} |X_j - X'_j|^q \right] \geq E_Q \left[ YY' e^{-t\|X_S - X_{Sc}\|_{q, \beta}^q} |X_j - X'_j|^q \right] - \vartheta_0(X_S, X_{Sc}) \cdot M_\mu(2M_X)^q.$$  \[28\]

and the analogue of Eq. (29) in the more general setting is similarly

$$E_Q \left[ YY' e^{-t\|X_S - X_{Sc}\|_{q, \beta}^q} \right] \geq E_Q \left[ YY' e^{-t\|X - X'\|_{q, \beta}^q} \right] - \vartheta_0(X_S, X_{Sc}).$$  \[29\]
As a consequence, we can now follow the proof of Theorem 2 and obtain the following general bound which holds without the need of independence assumption $X_S \perp X_{S^c}$:

$$\partial_{\beta_j} P_{ML}(\beta; Q) \geq \xi(\beta) \cdot |P_{ML}(\beta; Q)| - C \cdot \vartheta(X_S, X_{S^c})$$

where $C = M^2(2M_X)^q$.

This completes the proof of Theorem 2.

Theorem 1A’ allows a further direct generalization of Proposition 8 to the setting where the signal variables $X_S$ and noise variables $X_{S^c}$ are weakly dependent. We do not pursue further discussion on it for the space considerations.

F.2 Basic derivations for the metric learning objective

This section gives the derivation of the metric learning objective as appeared in Eq. (4). Let $X \in \mathbb{R}^p$ and $Y \in \{\pm 1\}$, and the loss $L(y, \hat{y}) = -y\hat{y}$. Write $k(x, x') = h(||x - x'||_q^q)$. Using the reproducing property of the RKHS, we have

$$F_n(\beta) = \min_f J_n(\beta, f)$$

where $J_n(\beta, f) = -\langle E[k(\beta^{1/q} \odot X, \cdot)Y], f \rangle_H + \lambda_n \|f\|_H^2$.

Note that $f \mapsto J_n(\beta, f)$ is quadratic in $f$ satisfying $J_n(\beta, f) = \lambda_n(\|f - \bar{f}\|_H^2 - \|\bar{f}\|_H^2)$ where $\bar{f} = \frac{1}{2\lambda_n} E[k(\beta^{1/q} \odot X, \cdot)Y]$ is the unique minimizer of $f \mapsto J_n(\beta, f)$. As a result, we obtain that $F_n(\beta) = J_n(\beta, \bar{f}) = -\lambda_n \|f\|_H^2$. Using the reproducing property again, we obtain that

$$F_n(\beta) = -\lambda_n \|\bar{f}\|_H^2 = -\frac{1}{4\lambda_n} E[k(\beta^{1/q} \odot X, \cdot)Y, \bar{E}[k(\beta^{1/q} \odot X', \cdot)Y']_H]$$

$$= -\frac{1}{4\lambda_n} E[YY'k(\beta^{1/q} \odot X, \beta^{1/q} \odot X')]_H.$$