Abstract

We propose a method for estimation in high-dimensional linear models with nominal categorical data. Our estimator, called SCOPE, fuses levels together by making their corresponding coefficients exactly equal. This is achieved using the minimax concave penalty on differences between the order statistics of the coefficients for a categorical variable, thereby clustering the coefficients. We provide an algorithm for exact and efficient computation of the global minimum of the resulting nonconvex objective in the case with a single variable with potentially many levels, and use this within a block coordinate descent procedure in the multivariate case. We show that an oracle least squares solution that exploits the unknown level fusions is a limit point of the coordinate descent with high probability, provided the true levels have a certain minimum separation; these conditions are known to be minimal in the univariate case. We demonstrate the favourable performance of SCOPE across a range of real and simulated datasets. An R package CatReg implementing SCOPE for linear models and also a version for logistic regression is available on CRAN.

1 Introduction

Categorical data arise in a number of application areas. For example, electronic health data typically contain records of diagnoses received by patients coded within controlled vocabularies and also prescriptions, both of which give rise to categorical variables with large numbers of levels [Jensen et al., 2012]. Vehicle insurance claim data also contain a large number of categorical variables detailing properties of the vehicles and parties involved [Hu et al., 2018]. When performing regression with such data as covariates, it is often helpful, both for improved predictive performance and interpretation of the fit, to fuse the levels of several categories together in the sense that the estimated coefficients corresponding to these levels have exactly the same value.

To fix ideas, consider the following ANOVA model relating response vector $Y \in \mathbb{R}^n$ to categorical predictors $X_{ij} \in \{1, \ldots, K_j\}$, $j = 1, \ldots, p$:

$$Y_i = \mu^0 + \sum_{j=1}^{p} \sum_{k=1}^{K_j} \theta_{jk}^0 1_{\{X_{ij} = k\}} + \varepsilon_i. \quad (1)$$
Here the $\varepsilon_i$ are independent zero mean random errors, $\mu^0$ is a global intercept and $\theta^0_{jk}$ is the contribution to the response of the $k$th level of the $j$th predictor; we will later place restrictions on the parameters to ensure they are identifiable. We are interested in the setting where the coefficients corresponding to any given predictor are clustered, so defining

$$s_j := |\{\theta^0_{j1}, \ldots, \theta^0_{jK_j}\}|$$

we have $s_j \ll K_j$, at least when $K_j$ is large. Note that our setup can include high-dimensional settings where $p$ is large and many of the predictors do not contribute at all to the response: when $s_j = 1$, the contribution of the $j$th predictor is effectively null as it may be absorbed by the intercept term.

1.1 Related work

Early work on collapsing levels together in low-dimensional models of the form (1) was based on performing a variety of significance tests for whether certain sets of parameters were equal [Tukey, 1949, Scott and Knott, 1974, Calinski and Corsten, 1985]. See also Delete or merge regressors [Maj-Kańska et al., 2015], a scheme involving agglomerative clustering based on $t$-statistics for differences between levels.

The CART algorithm [Breiman et al., 1984] for building decision trees effectively starts with all levels of the variables fused together and greedily selects which levels to split. One potential drawback of these greedy approaches is that in high-dimensional settings where the search space is very large, they may fail to find good groupings of the levels. The popular random forest procedure [Breiman et al., 1984] uses randomisation to alleviate the issues with the greedy nature of the splits, but sacrifices interpretability of the fitted model.

An alternative to greedy approaches in high-dimensional settings is using penalty-based methods such as the Lasso [Tibshirani, 1996]. This can be applied to continuous or binary data and involves optimising an objective for which global minimisation is computationally tractable, thereby avoiding some of the pitfalls of greedy optimisation. In contrast to random forest, the fitted models are sparse and interpretable. Inspired by the success of the Lasso and related methods for high-dimensional regression, a variety of approaches have proposed estimating $\theta^0 = (\theta^0_{j,k})_{j=1,...,p, k=1,...,K_j}$ and $\mu^0$ via optimising over $(\mu, \theta)$ a sum of a least squares criterion

$$\ell(\mu, \theta) := \frac{1}{2n} \sum_{i=1}^{n} \left( Y_i - \mu - \sum_{j=1}^{p} \sum_{k=1}^{K_j} \theta_{jk} 1\{X_{ij}=k\} \right)^2$$

and a penalty of the form

$$\sum_{j=1}^{p} \sum_{k=2}^{K_j} \sum_{l=1}^{k-1} w_{j,kl} |\theta_{jk} - \theta_{jl}|.$$

This is the CAS-ANOVA penalty of [Bondell and Reich, 2009]; see also [Gertheiss and Tutz, 2010, Chiquet et al., 2017]. The weights $w_{j,kl}$ can be chosen to balance the effects of having certain levels of categories more prevalent than others in the data. The penalty is an ‘all-pairs’ version of the fused Lasso [Tibshirani et al., 2005] and closely related to so-called convex clustering [Hocking et al., 2011]. We note that there are several other approaches besides using penalty functions. For instance [Pauger and Wagner, 2019] proposes a Bayesian modelling procedure using sparsity-inducing prior distributions to encourage fusion of levels. See also [Tutz and Gertheiss, 2016] and references therein for review of other methods including those based on mixture models and kernels.
The fact that the optimisation problem resulting from (4) is convex makes the procedure attractive. However, a potential drawback is that it may not always give a desirable form of shrinkage. Consider the case where $p = 1$, and dropping subscripts for simplicity, we have $K = 10$ levels. Furthermore, suppose all $w_{kl} = 1$, which would typically be the case if all levels were equally prevalent. Suppose these levels are clustered into 3 groups with $\theta_0^1 = \cdots = \theta_4^1 = -1$, $\theta_5^0 = \theta_6^0 = 0$ and $\theta_7^0 = \cdots = \theta_{10}^0 = 1$. Taking $\theta_k = \theta_k^0$ for all $k$, the penalty contribution in (4) is 48. If we were to split the middle group such that $-1 \leq \theta_5 < \theta_6 \leq 1$, the penalty contribution would only increase by $\theta_6 - \theta_5$, which is small relative to 48. In this case then, CAS-ANOVA will struggle to keep the middle group intact. We see this in Figure 1, which shows the result of applying CAS-ANOVA to data generated according to (1) with $p = 1$, $\theta_0$ as above, $n = 10$ (so we have a single observation corresponding to each level), and $\epsilon_i \sim N(0,1)$: there is no value of the tuning parameter $\lambda$ for which the estimates satisfy $\hat{\theta}_5 = \hat{\theta}_6$, with these distinct from the others.

As in the standard regression setting, the bias introduced by all-pairs $\ell_1$-type penalties may be reduced by choosing data-adaptive weights analogously to the adaptive Lasso [Zou, 2006], or replacing the absolute value $|\theta_{jk} + \theta_{jl}|$ by $\rho(|\theta_{jk} + \theta_{jl}|)$ where $\rho$ is a concave and non-decreasing penalty function [Oelker et al., 2015; Ma and Huang, 2017]. However, this does not address the issue of a preference for groups of unequal sizes. Additionally, optimising an objective involving a penalty with $O\left(\sum_{j=1}^p K_j^2\right)$ summands can be computationally challenging, both in terms of runtime and memory.

1.2 Overview of our contributions

To motivate the new approach we are proposing in this paper, let us consider the setting where the predictors are ordinal rather than nominal, so there is an obvious ordering among the levels. In these settings, it is natural to consider a fused Lasso penalty of the form

$$\sum_{j=1}^p \sum_{k=1}^{K_j-1} |\theta_{j\pi_j(k+1)} - \theta_{j\pi_j(k)}|,$$

where $\pi_j$ is a permutation of $\{1, \ldots, K_j\}$ specifying the given order [Gertheiss and Tutz, 2010]. If we treat the nominal variable setting as analogous to having ordinal variables with unknown orderings $\pi_j$, one might initially think of choosing $\pi_j$ corresponding to the order of the estimates.
\[ \mathbf{\theta}_j := (\theta_{jk})_{k=1}^{K_j}, \text{ such that } \theta_{j\pi_j(k)} = \theta_{j(k)}, \text{ where } \theta_{j(k)} \text{ is the } k\text{th smallest entry in } \mathbf{\theta}_j. \] 

This however leads to the ‘range’ penalty:

\[
\sum_{k=1}^{K_j-1} |\theta_{j(k+1)} - \theta_{j(k)}| = \max_{k} \theta_{jk} - \min_{k} \theta_{jk}. \tag{6}
\]

Whilst this shrinks the largest and smallest of the estimated coefficients together, the remaining coefficients lying in the open interval between these are unpenalised and so no grouping of the estimates is encouraged, as we observe in Figure 1; see also [Oelker et al., 2015] for a discussion of this issue in the context of ordinal variables.

Our solution is to replace the \(|\theta_{j(k+1)} - \theta_{j(k)}|\) terms in (6) with \(\rho(\theta_{j(k+1)} - \theta_{j(k)})\) for a concave (and nonconvex) non-decreasing penalty function \(\rho\). Note that whereas in conventional high-dimensional regression, the use of nonconvex penalties has been primarily motivated by a need to reduce bias in the estimation of large coefficients [Fan and Li, 2001], here the purpose is different: in our setting a nonconvex penalty is in fact even necessary for shrinkage to sparse solutions to occur (see Proposition 1).

In Section 2 we formally introduce our method, which we call SCOPE, standing for Sparse Concave Ordering & Penalisation Estimator. The nonconvex penalty coupled with minimising over permutations presents a significant computational challenge. However, by choosing \(\rho\) to be the minimax concave penalty (MCP) [Zhang, 2010], we show that using a new dynamic programming approach we introduce in Section 3, we can recover the global minimum of the resulting objective function exactly in the univariate case, i.e. when \(p = 1\). We then build this into a blockwise coordinate descent approach to tackle the multivariate setting.

In Section 4 we study the theoretical properties of SCOPE and give sufficient conditions for the estimator to coincide with the least squares solution with oracular knowledge of the level fusions in the univariate case. We use this result to show that the oracle least squares solution is a fixed point of our blockwise coordinate descent algorithm in the multivariate case. We use this result to show that the oracle least squares solution is a fixed point of our blockwise coordinate descent algorithm in the multivariate case. In Section 5 we outline some extensions of our methodology including a scheme for handling settings when there is a hierarchy among the categorical variables. Section 6 contains numerical experiments that demonstrate the favourable performance of our method compared to a range of competitors. We conclude with a discussion in Section 7. Further detail of our algorithm can be found in the Appendix. Additional information of the experiments in Section 6 and all proofs of technical results, can be found in the Supplementary material.

2 SCOPE methodology

Recall that our goal is to estimate parameters \((\mu^0, \mathbf{\theta}^0)\) in model (1). Let us first consolidate some notation. For any \(\mathbf{\theta} \in \mathbb{R}^{K_1} \times \cdots \times \mathbb{R}^{K_p}\), we define \(\mathbf{\theta}_j := (\theta_{jk})_{k=1}^{K_j} \in \mathbb{R}^{K_j}\). We will study the univariate setting where \(p = 1\) separately, and so it will be helpful to introduce some simplified notation for this case, dropping any extraneous subscripts. We thus write \(K \equiv K_1, X_1 \equiv X_{i1}\) and \(\rho \equiv \rho_1\). Additionally, we let \(Y_k\) denote the average of the \(Y_i\) with \(X_i = k\):

\[
Y_k = \frac{1}{n_k} \sum_{i=1}^{n} Y_i 1_{\{X_i = k\}}, \tag{7}
\]

where \(n_k = \sum_{i=1}^{n} 1_{\{X_i = k\}}\).

To ensure identifiability, we will assume for all \(j = 1, \ldots, p\) that

\[
g_j(\mathbf{\theta}_j) = 0, \text{ where } g_j(\mathbf{\theta}_j) = \sum_{k=1}^{K_j} n_{jk} \theta_{jk} \text{ and } n_{jk} = \sum_{i=1}^{n} 1_{\{X_{ij} = k\}}. \tag{8}
\]
Let $\Theta_j = \{\theta_j \in \mathbb{R}^{K_j} : g_j(\theta_j) = 0\}$, and let $\Theta = \Theta_1 \times \cdots \times \Theta_p$. We will construct estimators by minimising over $\mu \in \mathbb{R}$ and $\theta \in \Theta$ an objective function of the form

$$
\tilde{Q}(\mu, \theta) = \ell(\mu, \theta) + \sum_{j=1}^{p} \sum_{k=1}^{K_j-1} \rho_j(\theta_{j(k+1)} - \theta_{j(k)}),
$$

where $\ell$ is the least squares loss function (3) and $\theta_{j(1)} \leq \cdots \leq \theta_{j(K_j)}$ are the order statistics of $\theta_j$. We allow for different penalty functions $\rho_j$ for each predictor in order to help balance the effects of varying numbers of levels $K_j$. The identifiability constraint that $\theta \in \Theta$ ensures that the estimated intercept $\hat{\mu} := \arg \min_{\mu} \tilde{Q}(\mu, \theta)$ satisfies $\hat{\mu} = \sum_{i=1}^{n} Y_i / n$. We therefore define

$$
Q(\theta) = \frac{1}{2n} \sum_{i=1}^{n} \left( Y_i - \hat{\mu} - \sum_{j=1}^{p} \sum_{k=1}^{K_j} \theta_{jk} 1_{(X_{ij}=k)} \right)^2 + \sum_{j=1}^{p} \sum_{k=1}^{K_j-1} \rho_j(\theta_{j(k+1)} - \theta_{j(k)}). \tag{9}
$$

We will take the regularisers $\rho_j : [0, \infty) \to [0, \infty)$ in (9) to be concave (and nonconvex); as discussed in the introduction and formalised in Proposition 1 below, a nonconvex penalty is necessary for fusion to occur.

**Proposition 1.** Consider the univariate case with $p = 1$. Suppose the subaverages $(\bar{Y}_k)_{k=1}^{K}$ are all distinct, and that $\rho_1 \equiv \rho$ is convex. Then any minimiser $\hat{\theta}$ of $Q$ has $\hat{\theta}_k \neq \hat{\theta}_l$ for all $k \neq l$ such that $\hat{\theta}(1) < \bar{Y}_k < \hat{\theta}(K)$ or $\hat{\theta}(1) < \bar{Y}_l < \hat{\theta}(K)$.

There are several possibilities for the penalty $\rho$. However, for computational reasons which we discuss in Section 3.3 it turns out to be helpful to base $\rho$ on the MCP [Zhang, 2010]:

$$
\rho(x) = \rho_{\gamma,\lambda}(x) = \int_{0}^{\infty} \frac{x}{t} \left( 1 - \frac{t}{\gamma \lambda} \right)_+ dt,
$$

where $(u)_+ = u 1_{(u \geq 0)}$. This is a piecewise quadratic function with gradient $\lambda$ at 0 and flat beyond $\gamma \lambda$. In the multivariate case we take $\rho_j = \rho_{\gamma,\lambda_j}$ with $\lambda_j = \lambda \sqrt{K_j}$. This choice of scaling is motivated by requiring that when $\theta^0 = 0$ we also have $\hat{\theta} = 0$ with high probability; see Lemma 6 in the Supplementary material. We discuss the choice of the tuning parameters $\lambda$ and $\gamma$ in Section 3.3 but first turn to the problem of optimising (9).

### 3 Computation

In this section we include details of how SCOPE is computed. Section 3.1 motivates and describes the dynamic programming algorithm we use to compute global minimiser of the SCOPE objective, which is highly non-convex. Section 3.2 contains details of how this is used to solve the multivariate objective by embedding it within a blockwise coordinate descent routine. Discussion of practical considerations is contained in Section 3.3.

#### 3.1 Univariate model

We now consider the univariate case ($p = 1$) and explain how the solutions are computed. In this case, we may rewrite the least squares loss contribution to the objective function in the
following way.

\[
\frac{1}{2n} \sum_{i=1}^{n} \left( Y_i - \hat{\mu} - \sum_{k=1}^{K} \theta_k 1_{\{X_i = k\}} \right)^2 = \frac{1}{2n} \sum_{i=1}^{n} \sum_{k=1}^{K} 1_{\{X_i = k\}} (Y_i - \hat{\mu} - \theta_k)^2 \\
= \frac{1}{2n} \sum_{k=1}^{K} \sum_{i=1}^{n} 1_{\{X_i = k\}} (Y_i - \hat{\mu} - \theta_k)^2 \\
= \frac{1}{2} \sum_{k=1}^{K} w_k (\bar{Y}_k - \theta_k)^2 + \frac{1}{2n} \sum_{i=1}^{n} (Y_i - \hat{\mu})^2 - \frac{1}{2} \sum_{k=1}^{K} w_k \bar{Y}_k^2,
\]

where \( w_k = n_k/n \). Thus the optimisation problem can be written equivalently as (suppressing the dependence of the MCP \( \rho \) on tuning parameters \( \gamma \) and \( \lambda \))

\[
\hat{\theta} \in \arg \min_{\theta \in \Theta} \frac{1}{2} \sum_{k=1}^{K} w_k (\bar{Y}_k - \theta_k)^2 + \sum_{k=1}^{K-1} \rho (\theta_{k+1} - \theta_k).
\]

(10)

In fact, it is straightforward to see that the constraint that the solution lies in \( \Theta \) will be automatically satisfied, so we may replace \( \Theta \) with \( \mathbb{R}^K \). Two challenging aspects of the optimisation problem above are the presence of the nonconvex \( \rho \) and the order statistics. The latter however are easily dealt with using the result below, which holds more generally whenever \( \rho \) is a concave function.

**Proposition 2.** Consider the univariate optimisation (10) with \( \rho \) any concave function such that a minimiser \( \hat{\theta} \) exists. If for \( k, l \) we have \( \bar{Y}_k > \bar{Y}_l \), then \( \hat{\theta}_k \geq \hat{\theta}_l \).

This observation substantially simplifies the optimisation: after re-indexing such that \( \bar{Y}_1 \leq \bar{Y}_2 \leq \cdots \leq \bar{Y}_K \), we may re-express (10) as,

\[
\hat{\theta} \in \arg \min_{\theta \in \mathbb{R}^K} \left\{ \frac{1}{2} \sum_{k=1}^{K} w_k (\bar{Y}_k - \theta_k)^2 + \sum_{k=1}^{K-1} \rho (\theta_{k+1} - \theta_k) \right\}.
\]

(11)

This objective is now reminiscent of the Fused Lasso [Tibshirani et al., 2005], for which there exist efficient dynamic programming procedures to compute the solution [Johnson, 2013]. Following this line of work, we define

\[
f_1(\theta_1) = \frac{1}{2} w_1 (\bar{Y}_1 - \theta_1)^2 \\
f_k(\theta_k) = \min_{\theta_{k-1} \leq \theta_k} \left\{ f_{k-1}(\theta_{k-1}) + \rho(\theta_k - \theta_{k-1}) \right\} + \frac{1}{2} w_k (\bar{Y}_k - \theta_k)^2 \\
b_k(\theta_k) = \arg \min_{\theta_{k-1} \leq \theta_k} \left\{ f_{k-1}(\theta_{k-1}) + \rho(\theta_k - \theta_{k-1}) \right\}
\]

for \( k = 2, \ldots, K \). Whenever a minimiser is not unique, we will take it to be the smallest minimiser; note that as typically \( \hat{\theta} \) will be unique, this will not cause any issues. Observe now that \( \hat{\theta}_K \) is the minimiser of the univariate objective function \( f_K \). Furthermore, we have \( \hat{\theta}_K = b_K(\hat{\theta}_K) \), and more generally \( \hat{\theta}_k = b_{k+1}(\hat{\theta}_{k+1}) \) for \( k = 1, \ldots, K - 1 \).

In order to make use of these properties, we must be able to compute \( f_K \) and the \( b_k \) efficiently. This is where the simple piecewise quadratic form of the MCP-based penalty is crucial. Some important consequences of this are summarised in the following lemma.

**Lemma 3.** For each \( k \),
(i) $f_k$ is continuous, coercive and piecewise quadratic;

(ii) $b_k$ is piecewise linear;

(iii) For each $\theta_{k+1} \in \mathbb{R}$, if the minimiser $\bar{\theta}_k = \bar{\theta}_k(\theta_{k+1})$ of $\theta_k \mapsto f_k(\theta_k) + \rho(\theta_{k+1} - \theta_k)$ over $(-\infty, \theta_{k+1}]$ satisfies $\theta_k < \theta_{k+1}$, then $f_k$ must be differentiable at $\bar{\theta}_k$.

Properties (i) and (ii) above permit exact representation of $f_k$ and $b_k$ with finitely many quantities. The key task then is to form the collection of intervals and corresponding coefficients of quadratic functions for

$$g_k(\theta_{k+1}) := \min_{\theta_k : \theta_k \leq \theta_{k+1}} \{ f_k(\theta_k) + \rho(\theta_{k+1} - \theta_k) \}$$

given a similar piecewise quadratic representation of $f_k$; and also the same for the linear functions composing $b_k$. A piecewise quadratic representation of $f_{k+1}$ would then be straightforward to compute, and we can iterate this process. To take advantage of property (iii) above, in computing $g_k(\theta_{k+1})$ we can separately search for minimisers at stationary points in $(-\infty, \theta_{k+1}]$ and compare the corresponding function values with $f_k(\theta_{k+1})$; the fact that we need only consider potential minimisers at points of differentiability will simplify things as we shall see below.

Suppose $I_{k,1}, \ldots, I_{k,m(k)}$ are intervals that partition $\mathbb{R}$ (closed on the left) and $q_{k,1}, \ldots, q_{k,m(k)}$ are corresponding quadratic functions such that $f_k(\theta_k) = q_{k,r}(\theta_k)$ for $\theta_k \in I_{k,r}$. Let us write

$$\tilde{q}_{k,r}(\theta_k) = \begin{cases} q_{k,r}(\theta_k) & \text{if } \theta_k \in I_{k,r} \\ \infty & \text{otherwise.} \end{cases}$$

We may then express $f_k$ as $f_k(\theta_k) = \min_r \tilde{q}_{k,r}(\theta_k)$. We can also express the penalty $\rho = \rho_{\gamma,\lambda}$ in a similar fashion. Let

$$\tilde{\rho}_1(x) := -\gamma \lambda^2 \{ 1 - x/(\gamma \lambda) \}^2 / 2 + \gamma \lambda^2 / 2 \text{ if } 0 \leq x < \gamma \lambda \text{ and } \infty \text{ otherwise,}$$

$$\tilde{\rho}_2(x) := \gamma \lambda^2 / 2 \text{ if } x \geq \gamma \lambda \text{ and } \infty \text{ otherwise.}$$

Then $\rho(x) = \min_\gamma \tilde{\rho}_1(x)$ for $x \geq 0$. Let $D_k$ be the set of points at which $f_k$ is differentiable. We then have, using Lemma \[\text{III} \] (iii) that

$$g_k(\theta_{k+1}) = \min_{\theta_k : \theta_k \leq \theta_{k+1}} \{ \min_r \tilde{q}_{k,r}(\theta_k) + \min_t \tilde{\rho}_t(\theta_{k+1} - \theta_k) \}$$

$$= \min_{\theta_k \in D_k} \min_{\theta_k < \theta_{k+1}} \min_r \{ \tilde{q}_{k,r}(\theta_k) + \tilde{\rho}_t(\theta_{k+1} - \theta_k) \}, f_k(\theta_{k+1}) \}$$

$$= \min \{ \min_{r,t} \tilde{q}_{k,r}(\theta_k) + \tilde{\rho}_t(\theta_{k+1} - \theta_k) \}, f_k(\theta_{k+1}) \} \},$$

where $\tilde{\min}$ denotes the minimum if it exists and $\infty$ otherwise. The fact that in the inner minimisation we are permitted to consider only points in $D_k$ simplifies the form of

$$u_{k,r,t}(\theta_{k+1}) := \min_{\theta_k \in D_k} \min_{\theta_k < \theta_{k+1}} \{ \tilde{q}_{k,r}(\theta_k) + \tilde{\rho}_t(\theta_{k+1} - \theta_k) \}.$$
(closed on the left) and corresponding quadratic functions as \( J_{k,1}, \ldots, J_{k,n(k)} \) and \( p_{k,1}, \ldots, p_{k,n(k)} \) respectively.

In order to produce a representation of \( f_{k+1} \) for use in future iterations, we must express \( g_k \) as a collection of quadratics on disjoint intervals. To this end, define for \( x \in \mathbb{R} \) the active set at \( x \), \( A(x) = \{ r : x \in J_{k,r} \} \). Note that the endpoints of the intervals \( J_{k,r} \) are the points where the active set changes and it is thus straightforward to determine \( A(x) \) at each \( x \). Let \( r(x) \) be the index such that \( g_k(x) = p_{k,r(x)}(x) \). For large negative values of \( x \), \( A(x) \) will contain a single index and for such \( x \) this must be \( r(x) \). Consider also for each \( r \in A(x) \setminus \{ r(x) \} \), the horizontal coordinate \( x' \) of the first intersection beyond \( x \) (if it exists) between \( p_{k,r} \) and \( p_{k,r(x)} \); let \( N(x) \) denote the collection of all such tuples \((x', r)\). Given \( r(x), N(x) \) can be computed easily. The intersection set \( N(x) \) then in turn helps to determine the smallest \( x' > x \) where \( r(x') \neq r(x) \) changes, that is the next knot of \( g_k \) beyond \( x \), as we now explain. Suppose at a point \( x_{\text{old}} \), we have computed \( r_{\text{old}} = r(x_{\text{old}}) \). We set \( x_{\text{cur}} = x_{\text{old}} \) and perform the following.

1. Given \( r(x_{\text{cur}}) \), compute \( N(x_{\text{cur}}) \) and set \( (x_{\text{int}}, r_{\text{int}}) = \arg\min\{ x : (x, r) \in N(x_{\text{cur}}) \} \).

2. If there are no changes in the active set between \( x_{\text{cur}} \) and \( x_{\text{int}} \), we have found the next knot point at \( x_{\text{int}} \) and \( r_{\text{int}} = r(x_{\text{int}}) \).

3. If instead the active set changes, move \( x_{\text{cur}} \) to the leftmost change point. We have that \( r(x) = r_{\text{old}} \) for \( x \in [x_{\text{old}}, x_{\text{cur}}) \). To determine if \( r(x) \) changes at \( x_{\text{cur}} \), we check if
   
   (i) \( r_{\text{old}} \) leaves the active set at \( x_{\text{cur}} \), so \( r_{\text{old}} \notin A(x_{\text{cur}}) \), or
   
   (ii) \( r_{\text{new}} \) enters the active set at \( x_{\text{cur}} \) and 'beats' \( r_{\text{old}} \), so \( r_{\text{new}} \in A(x_{\text{cur}}) \setminus A(x_{\text{old}}) \) and \( p_{k,r_{\text{new}}}(x_{\text{cur}} + \epsilon) < p_{k,r_{\text{old}}}(x_{\text{cur}} + \epsilon) \) for \( \epsilon > 0 \) sufficiently small.

If either hold \( x_{\text{cur}} \) is a knot and \( r(x_{\text{cur}}) \) may be computed via \( r(x_{\text{cur}}) = \arg\min_{r} \{ p_{k,r}(x_{\text{cur}}) : r \in A(x_{\text{cur}}) \} \). If neither hold, we conclude that \( r(x_{\text{cur}}) = r_{\text{old}} \) and go to step 1 once more.

Hence we can proceed from one knot of \( g_k \) to the next by comparing the values and intersections of a small collection of quadratic functions, and thereby form a piecewise quadratic representation of \( g_k \) in a finite number of steps. The pieces of \( b_k \) may be computed in a similar fashion. We note there are several modifications that can speed up the algorithm: for example, for each \( r, u_{k,r,2} \) is a constant function where it is finite (see \( p_{k,3} \) in the figure), and these can be dealt with more efficiently. Figure 2 illustrates the steps outlined above; for further details including pseudocode see Section A.2 of the Appendix.

It seems challenging to obtain meaningful bounds on the number of computations that must be performed at each stage of this process in terms of parameters of the data. However, to give an indication of the scalability of this algorithm we ran a simple example with 3 true levels and found that with 50 categories the runtime was under \( 10^{-3} \) seconds; with 2000 categories it was still well under half a second. More details on computation time can be found in Sections S1.1 and S2.2 of the Supplementary material.

### 3.2 Multivariate model

Coordinate descent has been shown empirically to be a successful strategy for minimising objectives for high-dimensional regression with nonconvex penalties such as the MCP [Breheny and Huang, 2011] [Mazumder et al., 2011] [Breheny and Huang, 2015], and we take this approach here. Considering the multivariate case, we iteratively minimise the objective \( Q \) over \( \theta_j := (\theta_{jk})_{k=1}^{K_j} \in \Theta_j \) keeping all other parameters fixed. Then for a given \((\lambda, \gamma)\) and initial estimate \( \hat{\theta}^{(0)} \in \Theta \), we repeat the following until a suitable convergence criterion is met:
Figure 2: Illustration of the optimisation problem and our algorithm, to be interpreted with reference to steps 1, 2, 3 in the main text. Shading indicates regions where the active set, displayed at the bottom of the plot, is invariant, and vertical dotted lines signify changes. Dotted curves correspond to parts of quadratic functions lying outside their associated intervals.

At \( x_{\text{old}} \), we have \( r(x_{\text{old}}) = 1 \), \( A(x_{\text{old}}) = \{1, 2\} \) and \( N(x_{\text{old}}) = \{(x_{\text{int}}^{(1)}, 2)\} \). Since the active set changes between \( x_{\text{old}} \) and \( x_{\text{int}}^{(1)} \), we move \( x_{\text{cur}} \) to the first change point \( P \) and see none of (i), (ii) occur. We therefore return to step 1 and compute \( N(x_{\text{cur}}) \) which additionally contains \( (x_{\text{int}}^{(2)}, 2) \).

As the active set is unchanged between \( x_{\text{cur}} \) and \( x_{\text{int}}^{(2)} \) we have determined the next knot point \( x_{\text{int}}^{(2)} \) and minimising quadratic \( p_{k,3} \).

1. Initialise \( m = 1 \), and set for \( i = 1, \ldots, n \)

\[
R_i = Y_i - \hat{\mu} - \sum_{l=1}^{p} \sum_{k=1}^{K_l} \hat{\theta}^{(m-1)}_{lk} \mathbb{1}_{\{X_{il}=k\}}. \tag{12}
\]

2. For \( j = 1, \ldots, p \), compute

\[
R_i^{(j)} = R_i + \sum_{k=1}^{K_j} \hat{\theta}^{(m-1)}_{jk} \mathbb{1}_{\{X_{ij}=k\}} \quad \text{for each } i,
\]

\[
\hat{\theta}^{(m)}_j = \arg \min_{\theta_j \in \Theta_j} \left\{ \frac{1}{2n} \sum_{i=1}^{n} \left( R_i^{(j)} - \sum_{k=1}^{K_j} \theta_{jk} \mathbb{1}_{\{X_{ij}=k\}} \right)^2 + \left( \sum_{k=1}^{K_j} \rho_j (\theta_{j(k+1)} - \theta_{j(k)}) \right) \right\} \tag{13}
\]

\[
R_i = R_i^{(j)} - \sum_{k=1}^{K_j} \hat{\theta}^{(m)}_{jk} \mathbb{1}_{\{X_{ij}=k\}} \quad \text{for each } i.
\]

3. Increment \( m \to m + 1 \).

We define a blockwise optimum of \( Q \) to be any \( \hat{\theta} \in \Theta \), such that for each \( j = 1, \ldots, p \),

\[
\hat{\theta}_j \in \arg \min_{\theta_j \in \Theta_j} Q(\hat{\theta}_1, \ldots, \hat{\theta}_{j-1}, \theta_j, \hat{\theta}_{j+1}, \ldots, \hat{\theta}_p). \tag{14}
\]
This is equivalent to \( \hat{\theta} \) being a fixed point of the block coordinate descent algorithm above. Provided \( \gamma > 0 \), \( Q \) is continuous in \( \theta \). As a consequence of Tseng [2001, Theorem 4.1 (c)], provided the minimisers \( \hat{\theta}^{(m)}_j \) in (13) are unique for all \( j \) and \( m \) (which will invariably be the case when the data are realisations of continuous random variables), then all limit points of the sequence \( (\hat{\theta}^{(m)}_j)_{m=0}^{\infty} \) are blockwise optima.

To obtain blockwise optima, it is important that the update steps (13) compute the global minimum. In the next section, we outline a dynamic programming algorithm that computes the exact global optimum of the univariate problem. In Section 4, we give conditions for the oracle least squares estimate (16) to be globally optimal for the univariate problem and blockwise optimal for the multivariate problem.

### 3.3 Practicalities

In practice the block coordinate descent procedure described above must be performed over a grid of \((\gamma, \lambda)\) values to facilitate tuning parameter selection by cross-validation. In line with analogous recommendations for other penalised regression optimisation procedures [Breheny and Huang 2011, Friedman et al. 2010], we propose, for each fixed \( \gamma \), to iteratively obtain solutions for an exponentially decreasing sequence of \( \lambda \) values, warm starting each application of block coordinate descent at the solution for the previous \( \lambda \). It is our experience that this scheme speeds up convergence and helps to guide the resulting estimates to statistically favourable local optima, as has been shown theoretically for certain nonconvex settings [Wang et al., 2014].

The grid of \( \gamma \) values can be chosen to be fairly coarse as the solutions appear to be less sensitive to this tuning parameter; in fact fixing \( \gamma \in \{8, 32\} \) yields competitive performance across a range of settings (see Section 6). The choice \( \gamma \downarrow 0 \), which mimics the \( \ell_0 \) penalty, has good statistical properties (see Theorem 4 and following discussion). However the global optimum typically has a smaller basin of attraction and can be prohibitively hard to locate, particularly in low signal to noise ratio settings where larger \( \gamma \) tends to dominate.

### 4 Theory

In this section, we study the theoretical properties of SCOPE. Recall our model

\[
Y_i = \mu^0 + \sum_{j=1}^{p} \sum_{k=1}^{K_j} \theta_{jk}^0 1\{X_{ij}=k\} + \varepsilon_i
\]

for \( i = 1, \ldots, n \), where \( \theta^0 \in \Theta \). We will assume the errors \((\varepsilon_i)^n_{i=1}\) have mean zero, are independent and sub-Gaussian with parameter \( \sigma \). Let

\[
\Theta_0 = \{ \theta \in \Theta : \theta_{jk} = \theta_{jl} \text{ whenever } \theta_{jk}^0 = \theta_{jl}^0 \text{ for all } j \}
\]

and define the oracle least squares estimate

\[
\hat{\theta}^0 := \arg \min_{\theta \in \Theta_0} \frac{1}{2n} \sum_{i=1}^{n} \left( Y_i - \hat{\mu} - \sum_{j=1}^{p} \sum_{k=1}^{K_j} \theta_{jk} 1\{X_{ij}=k\} \right)^2.
\]

This is the least squares estimate of \( \theta^0 \) with oracular knowledge of which categorical levels are fused in \( \theta^0 \).
Note that in the case where the errors have equal variance \( v^2 \), the expected mean squared prediction error of \( \hat{\theta}^0 \) satisfies

\[
\mathbb{E} \left\{ \frac{1}{n} \sum_{i=1}^{n} \left( \hat{\mu} - \mu^0 + \sum_{j=1}^{p} \sum_{k=1}^{K_j} (\hat{\theta}^0_{jk} - \theta^0_{jk}) 1_{\{X_{ij} = k\}} \right)^2 \right\} \leq \frac{v^2}{n} \left( 1 + \sum_{j=1}^{p} (s_j - 1) \right),
\]

with equality when \( \hat{\theta}^0 \) is unique.

Our results below establish conditions under which \( \hat{\theta}^0 \) is a blockwise optimum \([14]\) of the SCOPE objective \( Q [9] \), or in the univariate case when this in fact coincides with SCOPE. The minimum differences between the signals defined for each \( j \) by

\[
\Delta(\theta^0_j) := \min_{k,l} \{|\theta^0_{jk} - \theta^0_{jl}| : \theta^0_{jk} \neq \theta^0_{jl}\},
\]

will play a key role. If all components of \( \theta^0_j \) are equal we take \( \Delta(\theta^0_j) \) to be \( \infty \). We also introduce

\[
n_{j,\min} = \min_{k} n_{jk}, \quad n_{j,\min} = \min_{k} \sum_{l} n_{jl}, \quad \text{and} \quad n_{j,\max} = \max_{k} \sum_{l} n_{jl};
\]

these latter two quantities are the minimum and maximum number of observations corresponding to a set of fused levels in the \( j \)th predictor respectively.

### 4.1 Univariate model

We first consider the univariate case, where as usual we will drop the subscript \( j \) for simplicity.

The following result establishes conditions for recovery of the oracle least squares estimate \([16]\).

**Theorem 4.** Consider the model \([15]\) in the univariate case, with \( p = 1 \). Suppose there exists \( \eta \in (0, 1] \) such that \( \eta/s \leq n_{j,\min}/n \leq n_{j,\max}/n \leq 1/\eta s \). Let \( \gamma_* = \min\{\gamma, \eta s\} \) and \( \gamma^* = \max\{\gamma, \eta s\} \). Suppose further that

\[
\Delta(\theta^0_j) \geq 3 \left( 1 + \sqrt{2/\eta} \right) \sqrt{\gamma \gamma^* \lambda}.
\]

Then with probability at least

\[
1 - 2 \exp \left( -\frac{n_{\min} \eta s \gamma_* \lambda^2}{8 \sigma^2} + \log(K) \right),
\]

the oracle least squares estimate \( \hat{\theta}^0 \) is the global optimum of \([9]\), so \( \hat{\theta} = \hat{\theta}^0 \).

For a choice of the tuning parameters \((\gamma, \lambda)\) with \( \gamma \leq \eta s \) and \( \lambda \) such that equality holds in \([18]\), we have, writing \( \Delta \equiv \Delta(\theta^0) \), that \( \hat{\theta} = \hat{\theta}^0 \) with probability at least

\[
1 - 2 \exp \left( -c \eta^2 n_{\min} \Delta^2 / \sigma^2 + \log(K) \right),
\]

where \( c \) is an absolute constant. The quantity \( \eta \) reflects how equal the number of observations in the true fused levels are: in settings where the prevalences of the underlying true levels are roughly equal, we would expect this to be closer to 1. Consider now an asymptotic regime where \( K, s \) and \( 1/\Delta \) are allowed to diverge with \( n \), and \( n_{\min} \approx n/K \), so all levels have roughly the same prevalence. Then in order for \( \hat{\theta} = \hat{\theta}^0 \) with high probability, we require \( n \gtrsim K \log(K) / \Delta^2 \). This requirement cannot be weakened for any estimator; this fact comes as a consequence of minimax lower bounds on mis-clustering errors in Gaussian mixture models \([\text{Lu and Zhou, 2016} \text{, Theorem 3.3}]\).
4.2 Multivariate model

When the number of variables is \( p > 1 \) then models can become high-dimensional, with ordinary least squares estimation failing to provide a unique solution. We will however assume that the solution for \( \theta \in \Theta_0 \) to

\[
\sum_{j=1}^{p} \sum_{k=1}^{K_j} \theta_{jk}^0 \mathbb{1}\{X_{ij}=k\} = \sum_{j=1}^{p} \sum_{k=1}^{K_j} \theta_{jk} \mathbb{1}\{X_{ij}=k\}
\]

is unique, which occurs if and only if the oracle least squares estimate (16) is unique. A necessary condition for this is that \( \sum_j (s_j - 1) < n \). Our result below provides a bound on the probability that the oracle least squares estimate is a blockwise optimum of the SCOPE objective \( Q \) with \( \rho_j = \rho_j, \lambda_j \). This much more meaningful than an equivalent bound for \( \hat{\theta}_0 \) to be a local optimum as the number of local optima will be enormous. In general though there may be several blockwise optima, and it seems challenging to obtain a result giving conditions under which our blockwise coordinate descent procedure is guaranteed to converge to \( \hat{\theta}_0 \). Our empirical results (Section 6) however show that the fixed points computed in practice tend to give good performance.

**Theorem 5.** Consider the model (15). Suppose that there exists \( \eta \in (0, 1] \) such that \( \eta/s_j \leq n_{j, \min}/n \leq n_{j, \max}/n \leq 1/\eta s_j \) for all \( j = 1, \ldots, p \). Let \( \gamma_j = \min\{\gamma_j, \eta s_j\} \) and \( \gamma_j^* = \max\{\gamma_j, \eta s_j\} \). Further suppose that

\[
\Delta(\theta_{j,0}) \geq 3 \left( \frac{4}{3} + \frac{\sqrt{2}}{\eta} \right) \sqrt{\gamma_j \gamma_j^* \lambda_j}.
\]

Then with probability at least

\[
1 - 4 \sum_{j=1}^{p} \exp \left( -\frac{n_{j,\min}\gamma_j s_j \lambda_j^2}{8\sigma^2} + \log(K_j) \right),
\]

the oracle least squares estimate \( \hat{\theta}_0 \) (16) is a blockwise optimum of (9).

This result follows from applying Theorem 4 to each of the \( j = 1, \ldots, p \) partial residuals at the oracle least squares estimate.

Now suppose \( \gamma_j \leq \eta s_j \) and \( \lambda_j \) are such that equality holds in (20) for all \( j \). Then writing \( K_{\max} = \max_j K_j \), \( n_{\min} = \min_j n_{j,\min} \) and \( \Delta_{\min} = \min_j \Delta(\theta_{j,0}) \), we have that \( \hat{\theta}_0 \) is a blockwise optimum of (9) with probability at least

\[
1 - 4 \exp \left( -c \eta^2 n_{\min} \Delta_{\min}^2 / \sigma^2 + \log(K_{\max} p) \right),
\]

where \( c \) is an absolute constant. Considering an analogous asymptotic regime to that described in the previous section for the univariate case where here \( n_{\min} \asymp n / K_{\max} \), we see that in order for \( \hat{\theta}_0 \) to be a blockwise optimum with high probability, it is sufficient that

\[
n \gtrsim K_{\max} \log(K_{\max} p) / \Delta_{\min}^2.
\]

5 Extensions

In this section, we describe some extensions of our SCOPE methodology.
Continuous covariates. If some of the covariates are continuous rather than categorical, we can apply any penalty function of choice to these, and perform a regression by optimising the sum of a least squares objective, our SCOPE penalty and these additional penalty functions, using (block) coordinate descent.

For example, consider the model \( \left[ \right] \) with the addition of \( d \) continuous covariates. Let \( Z \in \mathbb{R}^{n \times d} \) be the centred design matrix for these covariates with \( i \)th row \( Z_i \in \mathbb{R}^d \). One can fit a model with SCOPE penalising the categorical covariates, and the Lasso with tuning parameter \( \alpha > 0 \) penalising the continuous covariates, resulting in the following objective over \( \beta \in \mathbb{R}^d \) and \( \theta \in \Theta \):

\[
\frac{1}{2n} \sum_{i=1}^n \left( Y_i - \hat{\mu} - Z_i^T \beta - \sum_{j=1}^p \sum_{k=1}^{K_j} \theta_{jk} \mathbf{1}_{\{X_{ij} = k\}} \right)^2 + \alpha \| \beta \|_1 + \sum_{j=1}^p \sum_{k=1}^{K_j-1} \rho_j (\theta_{j(k+1)} - \theta_{j(k)}).
\]

This sort of integration of continuous covariates is less straightforward when attempting to use tree-based methods to handle categorical covariates, for example.

Generalised linear models. Sometimes a generalised linear model may be appropriate. Although a quadratic loss function is critical for our exact optimisation algorithm described in Section \ref{section:algorithm}, we can iterate local quadratic approximations to the loss term in the objective and minimise this. This results in a proximal Newton algorithm and is a version of the standard approach for solving \( \ell_1 \)-penalised generalised linear models \cite[Section 3]{Friedman2010}.

For the case of binary response, we apply this scheme to perform a logistic regression using tree-based methods to handle categorical covariates, for example.

Hierarchical categories. Often certain predictors may have levels that are effectively sub-divisions of the levels of other predictors. Examples include category of item in e-commerce or geographical data with predictors for continent, countries and district. For simplicity, we will illustrate how such settings may be dealt with by considering a case with two predictors, but is clear how this may be generalised to more complex hierarchical structures. Suppose there is a partition \( G_1 \cup \cdots \cup G_{K_1} \) of \( \{1, \ldots, K_2\} \) such that for all \( k = 1, \ldots, K_1 \),

\[
X_{i2} \in G_k \implies X_{i1} = k,
\]

so the levels of the second predictor in \( G_k \) represent subdivisions of \( k \)th level of the first predictor. Let \( K_{2k} := |G_k| \) and let \( \theta_{2k} \) refer to the subvector \( (\theta_{2l})_{l \in G_k} \) for each \( k = 1, \ldots, K_1 \), so components of \( \theta_{2k} \) are the coefficients corresponding to the levels in \( G_k \). Also let \( \theta_{2k(r)} \) denote the \( r \)th order statistic within \( \theta_{2k} \). It is natural to encourage fusion among levels within \( G_k \) more strongly than for levels in different elements of the partition. To do this we can modify our objective function so the penalty takes the form

\[
\sum_{k=1}^{K_1-1} \rho_1 (\theta_{1(k+1)} - \theta_{1(k)}) + \sum_{k=1}^{K_1} \sum_{l=1}^{K_{2k}-1} \rho_{2k} (\theta_{2k(l+1)} - \theta_{2k(l)}).
\]

We furthermore enforce the identifiability constraints that

\[
\sum_{l=1}^{K_1} n_{1l} \theta_{1l} = 0 \quad \text{and} \quad \sum_{l \in G_k} n_{2l} \theta_{2l} = 0 \quad \text{for all} \quad k = 1, \ldots, K.
\]

As well as yielding the desired shrinkage properties, an additional advantage of this approach is that the least squares criterion is separable in \( \theta_{21}, \ldots, \theta_{2K_1} \), so the blockwise update of \( \theta_2 \) can be performed in parallel. This can lead to a substantial reduction in computation time if \( K_2 \) is large.
6 Experiments

In this section we explore the empirical properties of SCOPE. We first present the results on the performance on simulated data, and then in Section 6.3 describe an analysis of US census data using SCOPE.

We denote SCOPE with a specific choice of $\gamma$ as SCOPE-$\gamma$, and SCOPE-CV denotes SCOPE with a cross-validated choice of $\gamma$. We compare SCOPE to linear or logistic regression where appropriate and a range of existing methods, including CAS-ANOVA [Bondell and Reich, 2009], and an adaptive version where the weights $w_{j,kl}$ are multiplied by a factor proportional to $|\hat{\theta}_{j,k}^{\text{init}} - \hat{\theta}_{j,l}^{\text{init}}|^{-1}$, where $\hat{\theta}_{j,k}^{\text{init}}$ is an initial CAS-ANOVA estimate. As well as this, we include Delete or merge regressors (DMR) [Maj-Kańska et al., 2015], Bayesian effect fusion (BEF) [Pauger and Wagner, 2019] and the Lasso [Tibshirani, 1996] in some experiments. Lastly, we also include comparison to tree-based approaches such as CART [Breiman et al., 1984] and Random forests (RF) [Breiman, 2001]. For full details of the specific versions of these methods used in the numerical experiments, see Section S2.1 of the Supplementary material.

6.1 Simulations

We simulated data according to the model (1) with the covariates $X_{ij}$ generated randomly in the following way. We first drew $(W_{ij})^{p}_{j=1}$ from a multivariate $N_p(0, \Sigma)$ distribution where the covariance matrix $\Sigma$ had ones on the diagonal. The off-diagonal elements of $\Sigma$ were chosen such that $U_{ij} := \Phi^{-1}(W_{ij})$ had $\text{corr}(U_{ij}, U_{ik}) = \rho$ for $j \neq k$. The marginally uniform $U_{ij}$ were then quantised to give $X_{ij} = \lceil 24U_{ij} \rceil$, so the number of levels $K_j = 24$.

The errors $\varepsilon_i$ were independently distributed as $N(0, \sigma^2)$. The performance of SCOPE and competitor methods was measured using mean squared prediction error on $10^5$ new (noiseless) observations generated in the same way as the training data, and final results are averages over 500 draws of training and test data. We considered various settings of $(n,p,\rho,\theta_0^0,\sigma^2)$ below with low-dimensional and high-dimensional scenarios considered in Sections 6.1.1 and 6.1.2 respectively. The coefficient vectors for each experiment are specified up to an additive constant, which is required to satisfy the identifiability condition (8).

6.1.1 Low-dimensional experiments

Results are presented for three settings with $n = 500$, $p = 10$ given below.

1. $\theta_j^0 = (-3, \ldots, -3, 0, \ldots, 0, 3, \ldots, 3)$ for $j = 1, 2, 3$, and $\theta_j^0 = 0$ otherwise; $\rho = 0$.

2. $\theta_j^0 = (-3, \ldots, -3, 0, \ldots, 0, 3, \ldots, 3)$ for $j = 1, 2, 3$, and $\theta_j^0 = 0$ otherwise; $\rho = 0$.

3. As Setting 1, but with $\rho = 0.8$.

Each of these experiments were performed with noise variance $\sigma^2 = 1, 6.25, 25$ and 100. Methods included for these experiments were SCOPE-8, SCOPE-32, SCOPE-CV, linear regression, vanilla and adaptive CAS-ANOVA, DMR, Bayesian effect fusion, CART and Random forests. Also included are the results from the oracle least squares estimator (16).

Results are shown in Figure 3 and further details are given in Section S2.2.1 of the Supplementary material. Across all experiments, SCOPE with a cross-validated choice of $\gamma$ exhibits prediction performance at least as good as the optimal approaches, and in all but the lowest noise settings performs better than the other methods that were included. In these exceptions,
we see that fixing $\gamma$ to be a small value (corresponding to high-concavity) provides leading performance.

In low noise settings, we see that the methods based on first estimating the clusterings of the levels and then estimating the coefficients without introducing further shrinkage, such as DMR or Bayesian effect Fusion, perform well. However these struggle when the noise is larger. In contrast the tree-based methods perform poorly in low noise settings but exhibit competitive performance in high-noise settings.

### 6.1.2 High-dimensional experiments

We considered 8 settings as detailed below, each with $n = 500$, $p = 100$ and simulated 500 times.

1. $\theta_j^0 = (-2, \ldots, -2, 0, \ldots, 0, 2, \ldots, 2)$ for $j = 1, 2, 3, \theta_j^0 = (-2, \ldots, -2, 0, \ldots, 0, 2, \ldots, 2)$ for $j = 4, 5, 6$, and $\theta_j^0 = 0$ otherwise; $\rho = 0$ and $\sigma^2 = 50$.

2. As Setting 1, but with $\rho = 0.5$.

3. $\theta_j^0 = (-2, \ldots, -2, 0, \ldots, 0, 2, \ldots, 2)$ for $j = 1, 2, 3, \theta_j^0 = (-2, \ldots, -2, 3, \ldots, 3)$ for $j = 4, 5, 6$, and $\theta_j^0 = 0$ otherwise; $\rho = 0.5$ and $\sigma^2 = 100$. 

---

**Figure 3:** Prediction performance of various methods: (A) SCOPE-8; (B) SCOPE-32; (C) SCOPE-CV; (D) Linear regression; (E) Oracle least squares; (F) CAS-ANOVA; (G) Adaptive CAS-ANOVA; (H) DMR; (I) BEF; (J) CART; (K) RF.
4. $\theta_j^0 = (\underbrace{-2, \ldots, -2}_5, \underbrace{-1, \ldots, -1}_4, \underbrace{0, \ldots, 0}_5, \underbrace{1, \ldots, 1}_5, \underbrace{2, \ldots, 2}_5)$ for $j = 1, \ldots, 5$, and $\theta_j^0 = 0$ otherwise; $\rho = 0$ and $\sigma^2 = 25$.

5. $\theta_j^0 = (\underbrace{-2, \ldots, -2}_8, \underbrace{3, \ldots, 3}_8)$ for $j = 1, \ldots, 25$, and $\theta_j^0 = 0$ otherwise; $\rho = 0$ and $\sigma^2 = 1$.

6. As Setting 5, but with $\rho = 0.5$.

7. $\theta_j^0 = (\underbrace{-2, \ldots, -2}_4, \underbrace{0, \ldots, 0}_6, \underbrace{2, \ldots, 2}_6)$ for $j = 1, \ldots, 10$, and $\theta_j^0 = 0$ otherwise; $\rho = 0$ and $\sigma^2 = 25$.

8. $\theta_j^0 = (\underbrace{-3, \ldots, -3}_6, \underbrace{-1, \ldots, -1}_6, \underbrace{1, \ldots, 1}_6, \underbrace{3, \ldots, 3}_6)$ for $j = 1, \ldots, 5$, and $\theta_j^0 = 0$ otherwise; $\rho = 0$ and $\sigma^2 = 25$.

Models were fitted using SCOPE-8, SCOPE-32, SCOPE-CV, DMR, CART, Random forests and the Lasso. Results are displayed in Figure 4; further details can be found in Section S2.2.2.

Figure 4: Prediction performance of various methods: (A) SCOPE-8; (B) SCOPE-32; (C) SCOPE-CV; (D) DMR; (E) CART; (F) RF; (G) Lasso.
of the Supplementary material.

Across all the settings in this study, SCOPE performs better than any of the other methods included. This is regardless of which of the three $\gamma$ regimes is chosen, although cross-validating $\gamma$ gives the strongest performance overall. Comparing the results for $\gamma = 8$ and $\gamma = 32$ suggests that a larger (low-concavity) choice of $\gamma$ is preferable for higher-dimensional settings. In settings 5 and 6, which have a high signal-to-noise ratio, a cluster of points at approximately zero can be seen in Figure 4. These experiments correspond to SCOPE obtaining the true underlying groupings of the coefficients, giving these striking results. In contrast, DMR which initially applies a group Lasso [Yuan and Lin, 2006] to screen the categorical variables and give a low-dimensional model necessarily misses some signal variables in this first stage and hence struggles here.

6.2 Real data analysis

The Adult Data Set, available from the UCI Machine Learning Repository [Dua and Graff, 2019], contains a sample of 45,222 observations based on information from the 1994 US census. The binary response variable is 0 if the individual earns at most $50,000 a year, and 1 if they earn more than $50,000 a year. There are 2 continuous variables and 8 categorical, some such as ‘native country’ with large numbers of levels, bringing the total dimension to 93. An advantage of using SCOPE here over black-box predictive tools such as Random forests is the interpretability of the fitted model.

In Table 1, we show the 25-dimensional fitted model. For example, within Education level, we see that six distinct levels have been identified. These agree almost exactly with the stratification one would expect, with all school dropouts before 12th grade being grouped together at the lowest level.

![Figure 5: Prediction performance and fitted model dimension (respectively) of various methods: (A) SCOPE-100; (B) SCOPE-250; (C) Logistic regression; (D) CAS-ANOVA; (E) Adaptive CAS-ANOVA; (F) DMR; (G) BEF; (H) CART; (I) RF.](image)

Here we assess performance in the challenging setting when the training set is quite small by randomly selecting 1% (452) of the total observations for training, and using the remainder as a test set. Any observations containing levels not in the training set were removed. Models were fitted with SCOPE-100, SCOPE-250, logistic regression, vanilla and adaptive CAS-ANOVA, DMR, Bayesian effect fusion, CART and Random forests.

We see that both SCOPE-100 and SCOPE-250 are competitive, with CART and Random forests also performing well, though the latter two include interactions in their fits. CAS-ANOVA also performs reasonably well but the long tail of the boxplot indicates that the average
### Table 1: Coefficients of SCOPE model trained on the full dataset.

| Variable          | Coefficient | Levels                                                                 |
|-------------------|-------------|-------------------------------------------------------------------------|
| Intercept         | −3.048      |                                                                        |
| Age               | 0.027       |                                                                        |
| Hours per week    | 0.029       |                                                                        |
| Work class        | 0.378       | Federal government, Self-employed (incorporated)                        |
|                   | 0.058       | Private                                                                 |
|                   | −0.143      | Local government                                                        |
|                   | −0.434      | Self-employed (not incorporated), State government, Without pay         |
| Education level   | 1.691       | Doctorate, Professional school                                          |
|                   | 1.023       | Master’s                                                                |
|                   | 0.640       | Bachelor’s                                                              |
|                   | −0.132      | Associate’s (academic), Associate’s (vocational), Some college (non-graduate) |
|                   | −0.546      | 12th, High school grad                                                  |
|                   | −1.539      | Preschool, 1st-4th, 5th-6th, 7th-8th, 9th, 10th, 11th                   |
| Marital status    | 0.059       | Divorced, Married (army forces spouse), Married (civilian spouse), Married (absent spouse), Widowed |
|                   | −0.476      | Never married                                                           |
| Occupation        | 0.560       | Executive/Managerial                                                    |
|                   | 0.311       | Professional/Specialty, Protective service, Tech support                |
|                   | −0.003      | Armed forces, Sales                                                    |
|                   | −0.168      | Admin/Clerical, Craft/Repair                                            |
|                   | −0.443      | Machine operative/inspector, Transport                                  |
|                   | −1.107      | Farming/Fishing, Handler/Cleaner, Other service, Private house servant  |
| Relationship*     | 1.498       | Wife                                                                    |
|                   | 0.332       | Husband                                                                 |
|                   | −1.220      | Not in family                                                           |
|                   | −1.482      | Unmarried, Other relative                                               |
|                   | −2.144      | Own child                                                               |
| Race              | 0.013       | White                                                                   |
|                   | 0.008       | Asian/Pacific islander, Other                                           |
|                   | −0.182      | Native-American/Inuit, Black                                            |
| Sex               | 0.139       | Male                                                                    |
|                   | −0.619      | Female                                                                  |
| Native country    | 0.018       | KH, CA, CU, ENG, FR, DE, GR, HT, HN, HK, HU, IN, IR, IE, IT, JM, JP, PH, PL, PT, PR, TW, US, YU |
|                   | −0.882      | CN, CO, DO, EC, SV, GT, NL, LA, MX, NI, GU-VI-etc, PE, SCT, ZA, TH, TT, VN |

misclassification error is a little larger than that of the best performers, and the fitted models are typically larger than those fitted by SCOPE.

### 6.3 Real data example with split levels

To create a more challenging example, we artificially created additional levels in the Adult Data Set as follows. For each categorical variable we recursively selected a level with probability proportional to its prevalence in the data and then split it into two by appending “-0” or “-1” to the level for each observation independently and with equal probabilities. We repeated this until the total number of levels reached \( m \) times the original number of levels for that variable for \( m = 2, 3, 4 \). This process simulates for example responses to a survey, where different respondents might answer ‘US’, ‘U.S.’, ‘USA’, ‘U.S.A.’, ‘United States’ or ‘United States of America’ to a question, which would naively all be treated as different answers.
We used 2.5% (1130) of the observations for training and the remainder for testing and applied SCOPE with $\gamma = 100$ and logistic regression. Results were averaged over 250 training and test splits. Figure 6 shows that as the number of levels increases, the misclassification error of SCOPE increases only slightly, whereas the fitted model dimension decreases slightly.

7 Discussion

In this work we have introduced a new penalty-based method for performing regression on categorical data. An attractive feature of a penalty-based approach is that it can be integrated easily with existing methods for regression with continuous data, such as the Lasso. Our penalty function is nonconvex, but in contrast to the use of nonconvex penalties in standard high-dimensional regression problems, the nonconvexity here is necessary in order to obtain sparse solutions, that is fusions of levels. Whilst computing the global optimum of nonconvex problems is typically very challenging, for the case with a single categorical variable with several hundred levels, our dynamic programming algorithm can solve the resulting optimisation problem in less than a few seconds on a standard laptop computer. The algorithm is thus fast enough to be embedded within a block coordinate descent procedure for handling multiple categorical variables.

Our work offers several avenues for further work. On the theoretical front, it would be interesting to obtain guarantees for block coordinate descent to converge to a good local optimum, a phenomenon that we observe empirically. On the methodology side, it would be useful to generalise the penalty to allow for clustering multivariate coefficient vectors; such clustering could be helpful in the context of mixtures of regressions models, for example.

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A Appendix

A.1 Candidate minimiser functions

We now write down the forms of the functions $p_{k,r}$ as defined in Section 3.1. We write $q_{k,r}(x) = a_rx^2 + b_rx + c_r$ for simplicity, suppressing the subscript $k$. For $S \subseteq \mathbb{R}$ and linear map $x \mapsto ax + b$, $aS + b$ denotes the set $\{ax + b : x \in S\}$.

Further recall from Section 3.1 the definition

$$u_{k,r,t}(\theta_{k+1}) = \min_{\theta_k \in D_k : \theta_k < \theta_{k+1}} \{\tilde{q}_{k,r}(\theta_k) + \tilde{\rho}_t(\theta_{k+1} - \theta_k)\}.$$ 

For a function $f : \mathbb{R} \rightarrow \mathbb{R} \cup \{\infty\}$, we denote the effective domain of $f$ by

$$\text{dom } f := \{x \in \mathbb{R} : f(x) < \infty\}.$$ 

For each $r = 1, \ldots, m(k)$, there are cases corresponding to $t = 1$ and $t = 2$. The formulas are as follows:

$$u_{k,r,1}(x) = \frac{2a_r x^2 + 2(b_r - 2a_r \gamma) x + (b_r - 2a_r \gamma)^2}{2(1 - 2a_r \gamma)} + c_r,$$

with $\text{dom } u_{k,r,1} = \begin{cases} (1 - 2a_r \gamma) I_{k,r} + \gamma (\lambda - b_r) & \text{if } 2a_r - 1/\gamma > 0 \\ \emptyset & \text{otherwise.} \end{cases}$

If $g_k(\theta_{k+1}) = u_{k,r,1}(\theta_{k+1})$, then

$$b_k(\theta_{k+1}) = \frac{\theta_{k+1} + \gamma(b_r - \lambda)}{1 - 2a_r \gamma}.$$ 

The second case is

$$u_{k,r,2}(x) = -\frac{b_r^2}{4a_r} + c + \frac{1}{2} \gamma \lambda^2,$$

with $\text{dom } u_{k,r,2} = \begin{cases} \left[-\frac{b_r}{2a_r} + \gamma \lambda, \infty\right] & \text{if } a_r > 0 \text{ and } -b_r/2a_r \in I_{k,r} \\ \emptyset & \text{otherwise.} \end{cases}$

Here, if $g_k(\theta_{k+1}) = u_{k,r,2}(\theta_{k+1})$, then

$$b_k(\theta_{k+1}) = -\frac{b_r}{2a_r}.$$ 

Lastly, observe that $g_k(\theta_{k+1}) \leq f_k(\theta_{k+1})$, and if $g_k(\theta_{k+1}) = f_k(\theta_{k+1})$, then clearly $b_k(\theta_{k+1}) = \theta_{k+1}$. Thus we also include each $\tilde{q}_{k,r}$ and $I_{k,r}$ for $r = 1, \ldots, m(k)$ as candidate minimiser functions.

A.2 Algorithm details

Algorithm 1 describes in detail how the optimisation routine works. In the algorithm we make use of the following objects (where $x, y \in \mathbb{R}$):

- $A(x)$ is a set of integers $r$ that index functions; this is the active set at $x$
- $E$ is a set of points $y$; this is the set of points at which the active set changes
- $N(x)$ is a set of tuples $(y, r)$, where $y$ is a point and $r$ is an integer; this is the intersection set at $x$
Algorithm 1 Outline of procedure for computing $f_k$

1: while $E, N(x) \neq \emptyset$ do
2:  if $\min\{y: (y, r) \in N(x)\} < \min E$ then
3:     $(y^*, r^*) = \arg\min\{y: (y, r) \in N(x)\}$
4:        $U = U \cup \{(\tilde{x}, y^*), r(x)\}$, $x = \tilde{x} = y^*$, $r(x) = r^*$
5:        $N(x) = \emptyset$, for any intersection between $p_{k-1, r(x)}$ and any $p_{k-1, r}$ with $r \in A(x) \setminus \{r(x)\}$
6:        at location $y > x$, set $N(x) = N(x) \cup \{(y, r)\}$.
7:  else
8:     $y^* = \min E$, $E = E \setminus \{y^*\}$,
9:        Update active set $A(y^*)$
10:    if $r(x) \notin A(y^*)$ then
11:        Set $r^*$ such that $p_{k-1, r^*} = \text{ChooseFunction}(A(y^*), y^*)$
12:           $U = U \cup \{(\tilde{x}, y^*), r(x)\}$, $x = \tilde{x} = y^*$, $r(x) = r^*$
13:           $N(x) = \emptyset$, for any intersection between $p_{k-1, r(x)}$ and any $p_{k-1, r}$ with $r \in A(x) \setminus \{r(x)\}$
14:           at location $y \geq x$, set $N(x) = N(x) \cup \{(y, r)\}$.
15:    else
16:        if $p_{k-1, r(x)} \neq p_{k-1, r^*} = \text{ChooseFunction}(A(y^*), y^*)$ then
17:           $U = U \cup \{(\tilde{x}, y^*), r(x)\}$, $x = \tilde{x} = y^*$, $r(x) = r^*$
18:           $N(x) = \emptyset$, for any intersection between $p_{k-1, r(x)}$ and any $p_{k-1, r}$ with $r \in A(x) \setminus \{r(x)\}$ at location $y > x$, set $N(x) = N(x) \cup \{(y, r)\}$.
19:        else
20:           if $A(y^*) \neq A(x)$ then
21:              For any intersection between $r(x)$ and any $r \in A(y^*) \setminus A(x)$ at location $y > x$,
22:                 set $N(y^*) = N(y^*) \cup \{(y, r)\}$
23:              For any $(y, r) \in N(x)$ with $r \notin A(y^*)$, set $N(y^*) = N(y^*) \setminus \{(y, r)\}$
24:                 $x = y^*$
25:           end if
26:        end if
27:    end if
28: end if
29: end while

Algorithm 2 ChooseFunction($H, x$)

Input: $H = \{h_1, \ldots, h_n\}$ a set of functions, $x$ a real number
1: Set $H_1 = \arg\min\{h(x): h \in H\}$
2: if $|H_1| = 1$ then
3:    Select $h^* \in H_1$
4: else
5:    Set $H_2 = \arg\min\{h'(x): h \in H_1\}$
6:    if $|H_2| = 1$ then
7:       Select $h^* \in H_2$
8:    else
9:       Set $H_3 = \arg\min\{h''(x): h \in H_2\}$
10:       Select $h^* \in H_3$ (choosing $h_i \in H_3$ with $i$ minimal if $|H_3| > 1$)
11: end if
12: end if

Output: $h^*$
• $U$ is a set of tuples $(I, r)$ where $I \subseteq \mathbb{R}$ is an interval and $r$ is an integer. Note that if $x = -\infty$ then $(x, y) = (-\infty, y)$.

All of the $p_{k,1}, \ldots, p_{k,m(k)}$ and $J_{k,m}$ are computed at the start of each iterate $k$. We then initialise

$$E = \bigcup_{r=1}^{n(k)} \partial J_{k-1,r}$$

the set of all of the end-points of the intervals $J_{k-1,1}, \ldots, J_{k-1,n(k)}$.

Here $x$ can be thought of as the ‘current position’ of the algorithm; $\tilde{x}$ is used to store when the minimising function $p_{k-1,r(x)}$ last changed. Initialise $\tilde{x} = -\infty$ and $x = -1 + \max\{y \in I_{k-1,1} : f'_{k-1}(y) \leq 0\}$. This choice of $x$ ensures that the active set $A(x)$ contains only one element (as mentioned in Section 3.1); this will always be the index corresponding to the function $\tilde{q}_{k-1,1}$.

We initialise the output set $U = \emptyset$, which by the end of this algorithm will be populated with the functions $\tilde{q}_{k,1}, \ldots, \tilde{q}_{k,m(k)}$ and their corresponding intervals $I_{k,1}, \ldots, I_{k,m(k)}$ that partition $\mathbb{R}$. Finally, we initialise the set $N(x)$ which will contain the intersections between $p_{k-1,r(x)}$ and other functions in the active set. As the active set begins with only one function, we set $N(x) = \emptyset$.

As mentioned in Section 3.1 there are several modifications that can speed up the algorithm. One such modification follows from the fact that for each $r$, $u_{k,r,2}$ is a constant function over its effective domain, and their effective domain is a semi-infinite interval (see Section A.1 of the Appendix for their expressions). Therefore, for a given point $x \in \mathbb{R}$, we can remove all such functions from $A(x)$ except for the one taking the minimal value.

We also note that in Algorithm 1 the set $N(x)$ is not recomputed in its entirety at every point $x$ at which $A(x)$ is updated, as is described in Section 3.1. Line 13 shows how sometimes $N(x)$ can instead be updated by adding or removing elements from it. Often, points 3 (i) and 3 (ii) from the description in the Section 3.1 will coincide, and in such instances some calls to ChooseFunction (Algorithm 2) can be skipped.
Supplementary material

This supplementary material is organised as follows. In Section S1 we include further details of our algorithm. Section S2 contains information regarding simulation settings and tables of results for the experiments in Section 6. The proofs of Proposition 1, Theorems 4 and 5 along with a number of lemmas they require can be found in Section S3.

S1 Additional algorithmic details

S1.1 Computation time experiments

The number of operations required for computing the univariate solution depends on the parameters $\gamma$ and $\lambda$, as well as the distribution of the entries in $\bar{Y}$. For example, if $\gamma$ is very large, then the complexity grows only quadratically in $K$. Theoretical runtime bounds are hard to obtain, since there exist choices of $f_k$ such that the number of pieces doubles when computing $f_{k+1}$. Thus, such an upper bound would yield only an exponential upper bound. However, such examples appear nor to exhibit the same behaviour in $f_{k+2}$; in practice we do not expect that runtime will grow exponentially in $K$.

A small experiment was performed to demonstrate the runtimes one can expect in practice. There were 3 settings; one with no signal, one with 2 true clusters and one with 5 true clusters. Independent and identically distributed Gaussian noise was added to each of the subaverages. As in Section 6.3 the number of categories was increased by random splitting of the levels. Each of these tests were repeated 25 times, on a computer with a 3.2GHz processor.

![Figure 7: Computation time for solving the univariate problem](image)

S1.2 Proofs of results

Proof of Proposition 2. Suppose, for a contradiction, that $\hat{\theta}_k < \hat{\theta}_l$. Then at least one of the following must be true:

$$|\hat{\theta}_k - \bar{Y}_k| > |\hat{\theta}_l - \bar{Y}_k|$$  \hspace{1cm} (22)

$$|\hat{\theta}_l - \bar{Y}_l| > |\hat{\theta}_k - \bar{Y}_l|.$$  \hspace{1cm} (23)

Let $\tilde{\theta}$ be defined as follows. Set $\tilde{\theta}_r = \hat{\theta}_r$ for all $r \neq k, l$. If (22) holds set $\tilde{\theta}_k = \hat{\theta}_l$ and if (23)
holds set \( \hat{\theta}_l = \hat{\theta}_k \). Observe that

\[
\sum_{r=1}^{n} \rho(\hat{\theta}_{(r+1)} - \hat{\theta}_{(r)}) \geq \sum_{r=1}^{n} \rho(\hat{\theta}_{(r+1)} - \hat{\theta}_{(r)})
\]

and that the squared loss of \( \hat{\theta} \) is strictly smaller than the squared loss of \( \hat{\theta} \), thus contradicting optimality of \( \hat{\theta} \).

\[\square\]

**Proof of Lemma** We proceed inductively, noting that the properties trivially hold for the base case \( f_1 \). Assume they hold for \( f_k \), then we prove these statements hold for \( g_k \), noting that then it is trivial to show them for \( f_{k+1} \). We begin by proving that \( g_k \) is continuous and coercive.

Clearly \( g_k(x) \geq \min f_k \) and as \( f_k \) is coercive, it follows that \( g_k(x) \to \infty \) as \( x \to -\infty \). As \( f_{k+1} = g_k + \frac{1}{2} w_{k+1}(x - \bar{Y}_{k+1})^2 \), it follows that \( f_{k+1} \) is coercive.

Considering some \( x_1 \in \mathbb{R} \), define

\[ y_*(x_1) = \arg \min_{y \leq x_1} f_k(y) + \rho(x_1 - y). \]

First see that for all values \( y \in (-\infty, x_1] \) we have \( f_k(y) + \rho(x - y) \) increasing continuously in \( x \) (\( \geq x_1 \)). This means that if \( y_* \) remains in this region then we are done. We also have from continuity of \( f_k \) and \( \rho \) that for all \( \varepsilon > 0 \), there exists \( \delta > 0 \) such that for all \( x \in [x_1, x_1 + \delta] \) that \( |f_k(x) + \rho(x_1 + \delta - x) - f_k(x_1)| < \varepsilon \). Since \( f_k(x_1) \geq f_k(y_*(x_1)) + \rho(x_1 - y_*(x_1)) \) it follows that for all such \( y \) we have

\[ |f(y_*(x)) + \rho(x - y_*(x)) - f(y_*(x_1)) - \rho(x_1 - y_*(x_1))| < \varepsilon, \]

thus \( g_k \) is continuous.

Now we turn to claim (iii). We show this by assuming that for all \( x \in \mathbb{R} \), \( f'_k(x-) \geq f'_k(x+) \) and then showing that this also holds for \( f_{k+1} \).

Suppose that we are increasing \( x \) and we have reached a point where \( f_{k+1}(y_*(x)) \) is not differentiable (that is, the left-derivative and the right-derivative do not match). We can assume that there is some window \( \delta > 0 \) such that \( y_*(t) \) is continuous for \( t \in (x - \delta, x) \) and such that \( f'_k(t) \) exists for this window. In particular we have by assumption that \( y_*(t) \) is linear for such \( t \). Note also by our inductive hypothesis we have \( f'_k(y_*(x_-)) \geq f'_k(y_*(x_+)) \) (we make use of this fact).

Note that for \( t \in (x - \delta, x) \), we have that \( y_*(t) = \alpha + \theta t \). Then \( f'_{k+1}(x_+) \) can be bounded above by \( f'_k(y_*(x_+)) + \rho(x - y_*(x)) \). Then for some sufficiently small \( \varepsilon > 0 \) we have

\[
f_{k+1}(x + \varepsilon) \leq f_k(y_*(x) + \varepsilon \theta) + \rho(x - y_*(x) - \varepsilon \theta) \leq f_{k+1}(x) + \varepsilon f'_{k+1}(x_-) + o(\varepsilon),
\]

where the last line follows from the basic definition of the right-hand derivative.

Now we use this to prove the claim. Because there are no points of \( f_k \) at which the left-derivative is less than the right-derivative, without loss of generality we claim that for all \( y \in \mathbb{R} \) that \( f_k \) is differentiable at \( y_*(x) \) unless \( y_*(x) = x \). Indeed, suppose not, then we have that \( f'_k(y_*(x_-)) > f'_k(y_*(x_+)) \) and necessarily that \( 0 \in \partial(f_k(\cdot) + \rho(x - \cdot)) \) at \( y_* \). But since our right-derivative of this function is less than our left we contradict the optimality of \( y_*(x) \) (as this point is in fact a local maxima).

Now we consider the remainder of claims (i) and (ii). In the case \( y_*(x) = x \), \( g_k(x) = f_k(x) \) so it follows that \( g_k \) is quadratic whenever this is true. It also holds trivially that \( y_*(x) = x \) is a linear function In the case \( y_*(x) < x \), then since \( f_k(\cdot) + \rho(x - \cdot) \) is piecewise quadratic (with two
pieces) then by claim (iii) it follows that $y_\ast(x)$ is linear in $x$, so $g_k(x) = f_k(y_\ast(x)) + \rho(x - y_\ast(x))$ is quadratic in $x$. We can conclude both that $g_k$ is a piecewise quadratic function (and therefore also $f_{k+1}$) and $b_k(x)$ is a piecewise linear function. As all of the claims are shown for $f_{k+1}$, the result follows.

\[ \Box \]

S2 Additional experimental information

S2.1 Details of methods

Tree-based methods

We used the implementation of Random forests \cite{Breiman2001} in the R package \texttt{randomForest} \cite{Liaw2002} with default settings. CART \cite{Breiman1984} was implemented in the R package \texttt{rpart} \cite{Therneau2019}, with pruning according to the 1-SE rule (described in the package documentation).

CAS-ANOVA

The CAS-ANOVA estimator $\hat{\theta}^{\text{cas}}$ optimises over $(\mu, \theta)$ a sum of a squared loss term (3) and an all-pairs penalty term (4). In particular, \cite{Bondell2009} consider two regimes of weight vectors $w$. The first is not data-dependent and sets $w_{j,k_1,k_2} = (K_j + 1)^{-1}n_{jk_1}n_{jk_2}$. The second, \textquote{adaptive CAS-ANOVA}, uses the ordinary least squares estimate for $\theta$ to scale the weights. Here, $w_{j,k_1,k_2} = (K_j + 1)^{-1}\sqrt{n_{jk_1}n_{jk_2}}|\hat{\theta}_{j,k_1}^{\text{OLS}} - \hat{\theta}_{j,k_2}^{\text{OLS}}|^{-1}$.

Here we introduce a new variant of adaptive CAS-ANOVA, following ideas in \cite{Buhlmann2011} for a 2-stage adaptive Lasso procedure. Instead of using the ordinary least squares estimate $\hat{\theta}_{j,k_1}^{\text{OLS}}$ in the above expression, an initial (standard) CAS-ANOVA estimate is used to scale the weights, with $\lambda$ selected for the initial estimate by 5-fold cross-validation. In simulations, this outperformed the adaptive CAS-ANOVA estimate using ordinary least squares initial estimates so in the interests of time and computational resources this was omitted from the simulation study. Henceforth adaptive CAS-ANOVA will refer to this 2-stage procedure.

The authors describe the optimisation of $\hat{\theta}^{\text{cas}}$ as a quadratic programming problem, which was solved using the R package \texttt{rosqp} \cite{Anderson2018}. Here we used our own implementation of the quadratic programming approach described by the authors. We found it considerably faster than the code available from the authors\’ website, and uses ADMM-based optimisation \cite{Boyd2011} tools not available at the time of its publication. We also found, as discussed in Section 5.1 of \cite{Maj-Kanska2015}, that we could not achieve the best results using the publicly available code. Lastly, using our own implementation allowed us to explore a modification of CAS-ANOVA using the more modern approach of adaptive weights via a 2-stage procedure \cite{Buhlmann2011} to compare SCOPE to a wider class of all-pairs penalty procedures.

For large categorical variables, solutions are slow to compute and consume large amounts of memory. In the case of binary response, CAS-ANOVA models were fitted iterating a locally quadratic approximation to the loss function.

DMR

The DMR algorithm \cite{Maj-Kanska2015} is implemented in the R package \texttt{DMRnet} \cite{Prochenka2018}. The degrees of freedom in the model is decided by 5-fold cross-validation. It is based on pruning variables using the Group Lasso \cite{Yuan2006} to obtain

3
at a low-dimensional model, then performing backwards selection based on ranking t-statistics for hypotheses corresponding to each fusion between levels in categorical variables.

The cross-validation routine appeared to error when all levels of all categorical variables were not present in one of the folds. In Section 6.2, cross-validation was therefore not possible so model selection was performed based on Generalized Information Criterion (GIC) [Zheng and Loh, 1995]. In all other examples, models were selected via 5-fold cross-validation.

**Bayesian effect fusion**

In Section 6.1.1 we include Bayesian effect fusion [Pauger and Wagner, 2019], implemented in the R package **effectFusion** [Pauger et al., 2019]. Coefficients within each categorical variable were modelled with a sparse Gaussian mixture model. The posterior mean was estimated with 1000 samples.

**Lasso**

In Section 6.1.2 we also include Lasso [Tibshirani, 1996] fits, to serve as a reference point. Of course, this is unsuitable for models where levels in categorical variables should be clustered together, but the advanced development of the well-known R package **glmnet** [Friedman et al., 2010] nevertheless sees its use in practice.

In order to make the fit symmetric across the categories within each variable, models were fitted with an unpenalised intercept and featuring dummy variables for all of the categories within each variable. This is instead of the corner-point dummy variable encoding of factor variables that is commonly used when fitting linear models.

**SCOPE**

For SCOPE, we have provided the R package **CatReg**. The univariate update step (see Section 3.1) is implemented in C++ using Rcpp [Eddelbuettel and François, 2011], with models fitted using a wrapper in R. For the binary response case, the outer loop to iterate the local quadratic approximations in the proximal Newton algorithm are done within R. In the future, performance could be improved by iterating the univariate update step (and the local quadratic approximations, as in Sections 6.2 and 6.3) within some lower-level language. In higher-dimensional experiments, SCOPE was slowed by cycling through all the variables; an active-set approach to this could make it faster still.

Speed could be improved further for very large-scale problems if we allow coefficients to take values in some finite grid, rather than any real value. The convergence behaviour and statistical properties of this approximate discrete version are not yet clear.

**S2.2 Further details of numerical experiments**

For the experiments in Section 6.1, we define the signal-to-noise ratio (SNR) as $\sigma_S/\sigma$, where $\sigma_S$ is the standard deviation of the signal $Y - \varepsilon$, and $\sigma$ is the standard deviation of the noise $\varepsilon$.

**S2.2.1 Low-dimensional simulations**

In Table 2 we include the mean squared prediction error (MSPE) from the experiments in Section 6.1.1. Table 3 contains details of computation time and dimension of the fitted models.
### Table 2: Mean squared prediction error (MSPE)

| Method      | Setting 1 | Setting 2 |
|-------------|-----------|-----------|
|             | $\sigma^2$: |         | $\sigma^2$: |         |
|             | 1 | 6.25 | 25 | 100 | 1 | 6.25 | 25 | 100 |
| SCOPE-8     | 0.014 | 0.450 | 4.571 | 12.936 | 0.015 | 0.285 | 6.775 | 12.697 |
| SCOPE-32    | 0.018 | 0.878 | 4.151 | 12.356 | 0.019 | 0.655 | 5.026 | 12.037 |
| SCOPE-CV    | 0.015 | 0.407 | 4.120 | 12.513 | 0.016 | 0.292 | 5.005 | 12.444 |
| Linear regression | 0.851 | 5.317 | 21.503 | 86.745 | 0.869 | 5.406 | 21.216 | 85.439 |
| Oracle least squares | 0.014 | 0.091 | 0.333 | 1.405 | 0.014 | 0.088 | 0.336 | 1.532 |
| CAS-ANOVA   | 0.617 | 1.602 | 5.448 | 14.814 | 1.483 | 1.626 | 5.466 | 13.421 |
| Adaptive CAS-ANOVA | 0.135 | 0.880 | 5.076 | 22.896 | 0.134 | 0.912 | 5.355 | 22.213 |
| DMR         | 0.014 | 0.448 | 4.884 | 18.394 | 0.016 | 0.409 | 6.430 | 17.457 |
| BEF         | 0.020 | 2.209 | 6.297 | 21.927 | 0.019 | 1.055 | 8.183 | 18.236 |
| CART        | 3.841 | 5.099 | 13.219 | 22.431 | 5.530 | 7.457 | 13.280 | 18.198 |
| RF          | 9.621 | 10.944 | 13.217 | 16.344 | 8.947 | 9.747 | 11.249 | 13.646 |

### Table 3: Mean fitted model dimension and computation time for the various methods.

| Method      | Mean fitted model dimension | Mean computation time (s) |
|-------------|----------------------------|---------------------------|
|             | $\sigma^2$: | 1 | 6.25 | 25 | 100 | Mean fitted model dimension | 1 | 6.25 | 25 | 100 | Mean computation time (s) |
| SCOPE-8     | 7.2 | 8.5 | 4.7 | 4.3 | 16 |
| SCOPE-32    | 9.6 | 12.6 | 13.2 | 9.8 | 48 |
| SCOPE-CV    | 7.9 | 10.3 | 16.8 | 10.9 | 68 |
| Oracle least squares | 7.0 | 7.0 | 7.0 | 7.0 | 0.00 |
| Linear regression | 231.0 | 231.0 | 231.0 | 231.0 | 0.01 |
| CAS-ANOVA   | 35.2 | 70.0 | 74.3 | 52.4 | 4679 |
| Adaptive CAS-ANOVA | 13.4 | 31.3 | 36.9 | 32.5 | 9659 |
| DMR         | 7.0 | 7.2 | 5.3 | 2.7 | 21 |
| BEF         | 7.3 | 6.3 | 4.1 | 2.0 | 975 |
| CART        | 4.336 | 5.685 | 9.910 | 18.543 | 0.01 |
| RF          | 4.039 | 5.673 | 9.157 | 13.766 | 0.66 |
S2.2.2 High-dimensional simulations

Table 4 contains mean squared prediction error of the experiments in Section 6.1.2. Now we include both computation time (Table 5) and fitted model dimension (Table 6) for the high-dimensional experiments.

| Method       | Setting: 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|--------------|------------|---|---|---|---|---|---|---|
| SCOPE-8      | 14.308     | 15.407 | 30.286 | 7.057 | 99.071 | 8.368 | 15.847 | 11.080 |
| SCOPE-32     | **13.956** | **10.751** | **22.034** | 6.879 | 65.348 | 0.062 | **14.816** | 11.234 |
| SCOPE-CV     | 14.038     | 10.837 | 22.330 | **6.856** | **52.449** | **0.058** | 14.855 | **11.000** |
| DMR          | 18.126     | 22.725 | 43.231 | 9.538 | 139.020 | 215.000 | 19.290 | 11.529 |
| CART         | 18.159     | 31.308 | 59.217 | 10.472 | 139.442 | 611.498 | 19.007 | 23.744 |
| RF           | 16.214     | 16.292 | 31.769 | 8.759 | 128.604 | 265.772 | 17.206 | 19.806 |
| Lasso        | 18.187     | 20.793 | 39.973 | 9.996 | 130.980 | 142.571 | 18.454 | 21.767 |

Table 4: Mean squared prediction error (MSPE)

Table 5: Mean computation time (s)

| Method       | Setting: 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|--------------|------------|---|---|---|---|---|---|---|
| SCOPE-8      | 224        | 322 | 348 | 76 | 234 | 518 | 209 | 175 |
| SCOPE-32     | 134        | 341 | 502 | 51 | 283 | 650 | 113 | 161 |
| SCOPE-CV     | 951        | 1739 | 2450 | 332 | 1516 | 2892 | 767 | 902 |
| DMR          | 26         | 38  | 39  | 26 | 30  | 36  | 30  | 29  |
| CART         | 0.1        | 0.1 | 0.1 | 0.0 | 0.1 | 0.1 | 0.1 | 0.1 |
| RF           | 5.7        | 5.7 | 5.9 | 2.7 | 5.8 | 5.8 | 5.8 | 5.8 |
| Lasso        | 1.5        | 1.5 | 1.6 | 1.2 | 1.4 | 1.5 | 1.5 | 1.5 |

Table 5: Mean computation time (s)

Table 6: Mean fitted model dimension

S2.2.3 Real data experiments

Table 7 contains the results from the experiments in Section 6.2.

| Method       | Misclassification error | Model dimension | Computation time (s) |
|--------------|------------------------|-----------------|----------------------|
| SCOPE-100    | 0.194                  | 10.5            | 467                  |
| SCOPE-250    | **0.191**              | 11.8            | 450                  |
| Logistic regression | 0.202                 | 68.9            | 0.04                 |
| CAS-ANOVA    | 0.198                  | 21.5            | 429                  |
| Adaptive CAS-ANOVA | 0.205                | 11.7            | 8757                 |
| DMR          | 0.235                  | 6.9             | 11                   |
| BEF          | 0.207                  | 9.8             | 1713                 |
| CART         | 0.196                  | 0.01            |                      |
| RF           | 0.194                  | 0.14            |                      |

Table 7: Mean misclassification errors and model dimension
S3 Proofs and technical results

S3.1 Proof of Proposition 1

Suppose that there exists \( l \neq k \) such that \( \hat{\theta}_k = \hat{\theta}_l \). Without loss of generality we have that \( \bar{Y}_k \neq \hat{\theta}_k \) (if \( \bar{Y}_k = \hat{\theta}_k \) then \( \bar{Y}_l = \hat{\theta}_l \) and it can be seen that \( \hat{\theta}^{(1)}_1 < \bar{Y}_l < \hat{\theta}_K \), in which case swap labels).

Now we construct \( \tilde{\theta} \) by setting \( \tilde{\theta}_r = \hat{\theta}_r \wedge \bar{Y}_k \) for \( r = 1, \ldots, k \), and \( \tilde{\theta}_r = \hat{\theta}_r \) otherwise. We have \( \ell(\hat{\mu}, \tilde{\theta}) < \ell(\hat{\mu}, \hat{\theta}) \) and, by convexity of \( \rho \), it follows that

\[
\sum_{r=1}^{K-1} \rho(\hat{\theta}_{r+1} - \hat{\theta}_r) \leq \sum_{r=1}^{K-1} \rho(\tilde{\theta}_{r+1} - \tilde{\theta}_r).
\]

This gives the conclusion \( Q(\tilde{\theta}) < Q(\hat{\theta}) \), contradicting the optimality of \( \hat{\theta} \).

S3.2 Proof of Theorem 4

The proof of Theorem 4 requires a number of auxiliary lemmas, which can be found in Section S3.2.1 of the Supplementary material.

We will work on the event that for \( k = 1, \ldots, K \),

\[
\left| \frac{1}{n_k} \sum_{i=1}^{n} \varepsilon_i 1_{\{X_i=k\}} \right| < \frac{1}{2} \sqrt{n \gamma_s \lambda}.
\]

Since \( \varepsilon \) is sub-Gaussian with parameter \( \sigma \), this event occurs with probability at least

\[
1 - 2 \sum_{k=1}^{K} \exp \left( -\frac{n w_k \gamma_s \lambda^2}{8 \sigma^2} \right) \geq 1 - 2 \exp \left( -\frac{n w_{\min} \gamma_s \lambda^2}{8 \sigma^2} + \log(K) \right),
\]

where we have used a union bound (and recall that \( w_k = n_k / n \)). It follows that \( \| \bar{Y} - \theta^0 \|_\infty < \sqrt{n \gamma_s \lambda} / 2 \), where \( \bar{Y} \in \mathbb{R}^K \) is the vector \((\bar{Y}_1, \ldots, \bar{Y}_K)^T\).

The indices can be relabelled such that \( \bar{Y}_1 \leq \cdots \leq \bar{Y}_K \), and it immediately follows from Proposition 2 that \( \hat{\theta}_1 \leq \cdots \leq \hat{\theta}_K \). Since \( \| \bar{Y} - \hat{\theta}^0 \|_\infty < \sqrt{n \gamma_s \lambda} / 2 \), it follows from assumption (18) that

\[
\theta^0_1 = \cdots = \theta^0_{k_1} < \theta^0_{k_1+1} = \cdots = \theta^0_{k_2} < \cdots < \theta^0_{k_s-1+1} = \cdots = \theta^0_{k_s},
\]

where we define \( k_0 = 0 \) for convenience. Indeed, observe that for \( j = 1, \ldots, s - 1 \), we have by the triangle inequality and (18) that

\[
\bar{Y}_{k_j+1} - \bar{Y}_{k_j} > 3 \left( 1 + \frac{\sqrt{2}}{\eta} \right) \sqrt{n \gamma^2 \lambda} > \gamma \lambda + 2(\sqrt{2s / n} \sqrt{\gamma \lambda} + \gamma \lambda) + 2 \sqrt{n \gamma_s \lambda}.
\]

It follows from Lemma 7 that \( \hat{\theta}_{k_j+1} - \hat{\theta}_{k_j} \geq \gamma \lambda \) for \( j = 1, \ldots, s - 1 \), enabling us to rewrite
the optimised objective:

$$Q(\hat{\theta}) = \frac{1}{2} \sum_{k=1}^{K} w_k (\bar{Y}_k - \hat{\theta}_k)^2 + \sum_{k=1}^{K-1} \rho(\hat{\theta}_{k+1} - \hat{\theta}_k)$$

$$= \frac{1}{2} \sum_{k=1}^{K} w_k (\bar{Y}_k - \hat{\theta}_k)^2 + \sum_{l=1}^{s} \sum_{k=k_{l-1}+1}^{k_l-1} \rho(\hat{\theta}_{k+1} - \hat{\theta}_k) + \frac{s-1}{2} \gamma \lambda^2$$  \hspace{1cm} (25)

$$= \min_{\theta \in \mathbb{R}^K} \frac{1}{2} \sum_{k=1}^{K} w_k (\bar{Y}_k - \theta_k)^2 + \sum_{l=1}^{s} \sum_{k=k_{l-1}+1}^{k_l-1} \rho(\theta_{k+1} - \theta_k) + \frac{s-1}{2} \gamma \lambda^2. \hspace{1cm} (26)$$

Note that (26) is separable in $\theta$ between true levels $l = 1, \ldots, s$ and thus they can be optimised separately. If $s = 1$, i.e. the true signal is zero, then the result follows from Lemma 9. Now we see what happens when $s > 1$.

Without loss of generality, consider $l = 1$ and note that if $k_1 = 1$, our $\hat{\theta}_1 = \hat{\theta}_0^1$. Hence, we can assume that $k_1 > 1$. We note that $\hat{\theta}_0^1 = \sum_{k=1}^{k_1} w_k Y_k/w_1^0$. We see that our goal is to compute

$$\arg \min_{\tilde{\theta} \in \mathbb{R}^{k_1}} \frac{1}{2} \sum_{k=1}^{k_1} w_k (\tilde{Y}_k - \tilde{\theta}_k)^2 + \sum_{l=1}^{s} \sum_{k=k_{l-1}+1}^{k_l-1} \rho(\theta_{k+1} - \theta_k)$$

$$= \hat{\theta}_1^0 + \arg \min_{\tilde{\theta} \in \mathbb{R}^{k_1}} \frac{1}{2} \sum_{k=1}^{k_1} w_k (\tilde{Y}_k - \tilde{\theta}_k)^2 - \sum_{l=1}^{s} \sum_{k=k_{l-1}+1}^{k_l-1} \rho(\tilde{\theta}_{k+1} - \tilde{\theta}_k).$$  \hspace{1cm} (27)

In the above expression, we define $\tilde{Y}$ and $\tilde{\theta}$ (both in $\mathbb{R}^{k_1}$) by

$$\tilde{Y}_k := Y_k - \hat{\theta}_1^0$$

$$\tilde{\theta}_k := \theta_k - \hat{\theta}_1^0$$

respectively for $k = 1, \ldots, k_1$. Note that we subtract $\hat{\theta}_1^0$ to ensure that the identifiability constraint (8) is satisfied on this subproblem (27). We have by assumption that for $k \in 1, \ldots, k_1$, $|\bar{Y}_k| \leq \sqrt{\eta \lambda} s \omega^0 \gamma / 2 \leq (2 \sqrt{\omega_0^0} \gamma \lambda / w_1^0$. Thus, Lemma 9 can be applied with $\tilde{\omega} = w_1^0$ and it follows that $\hat{\theta}_k = \hat{\theta}_1^0$ for $k = 1, \ldots, k_1$.

\[ \square \]

### S3.2.1 Auxiliary lemmas

Here we prove a number of results required to obtain conditions for recovering the oracle least squares estimate in the univariate case. Lemma 9 gives conditions for recovery of the true solution, in the case where there is zero signal. Lemmas 7 and 8 ensure that the true levels are far enough apart that they can be separated. Once we have this separation, we apply Lemma 9 on each of the levels to obtain the solution.

**Lemma 6.** Consider the optimisation problem

$$x^* = \arg \min_{x \geq 0} \frac{K}{2} (2\tau - x)^2 + \rho(x),$$

where $\tau > 0$ and $\kappa \in (0, 1]$. Suppose further that $\tau < (1 \wedge \sqrt{\kappa}) \lambda / 2\kappa$. Then $x^* = 0$ is the unique optimum.
Proof. We first observe that
\[ x^* = \arg \min_{x \geq 0} \frac{\kappa}{2} (2\tau - x)^2 + \rho_{\gamma,\lambda}(x) = \arg \min_{x \geq 0} \frac{1}{2} (2\tau - x)^2 + \rho_{\kappa,\gamma,\lambda}(x). \]

For convenience, we define \( F(x) := (2\tau - x)^2/2 + \rho_{\kappa,\gamma,\lambda}(x) \). It now suffices to show that \( F \) is uniquely minimised at 0 provided \( \tau < (1 + \sqrt{\kappa})/2\kappa \). We can clearly see that \( x^* \in [0, 2\tau] \).

Equation (2.3) of [Breheny and Huang 2011] gives the result when \( \kappa \gamma \geq 1 \).

When \( \kappa \gamma < 1 \), we see that any stationary point of \( F \) in \([0, \gamma \lambda \wedge 2\tau]\) must be a maximum. Therefore its minimum over \([0, \gamma \lambda]\) is attained at either \( x = 0 \) or \( x = \gamma \lambda \wedge 2\tau \). If \( 2\tau \leq \gamma \lambda \), then it suffices to check that \( F(0) < F(2\tau) \). This holds if and only if \( \tau < \gamma \lambda / (\gamma \kappa + 1) \), but since we are assuming \( \tau \leq \gamma \lambda / 2 \) and \( \kappa \gamma < 1 \), this is always satisfied.

If \( \gamma \lambda < 2\tau \), then we can see that the minimum of \( F \) over \([\gamma \lambda, 2\tau]\) will be attained at exactly \( 2\tau \). Thus, here it also suffices to check \( F(0) < F(2\tau) \), which holds if and only if \( \tau < \sqrt{\gamma / \kappa \lambda} / 2 \). The final bound \( \tau < (1 + \sqrt{\kappa})/2\kappa \) follows from combining the results for these cases.

The following is a deterministic result to establish separation between groups of coefficients.

**Lemma 7.** Consider the setup of Theorem 4. Suppose that \( \hat{Y}_1 \leq \cdots \leq \hat{Y}_K \), and that for \( j = 1, \ldots, s \) we have
\[ \hat{Y}_{k_j} - \hat{Y}_{k_{j-1}+1} < \sqrt{\bar{\eta}_j s} \lambda, \]
where \( k_j \) and \( k_{j-1} \) are as defined in (24). Suppose further that for \( j = 1, \ldots, s-1, \)
\[ \hat{Y}_{k_{j+1}} - \hat{Y}_{k_j} \geq \gamma \lambda + 2(\sqrt{2s/\bar{\eta}} \lambda \vee \gamma \lambda) + 2\sqrt{\bar{\eta}_j s} \lambda. \]

Then for \( j = 1, \ldots, s \), we have \( \hat{Y}_{k_{j+1}+1} \leq \hat{\theta}_{k_{j+1}} \leq \hat{\theta}_{k_j} \leq \hat{Y}_{k_j} \).

**Proof.** For convenience, within this lemma we define \( \zeta := \sqrt{\bar{\eta}_j s} \lambda \). Recall that the objective function which \( \hat{\theta} \) optimises takes the form
\[ Q(\theta) = \frac{1}{2} \sum_{k=1}^{K} w_k (\bar{Y}_k - \theta_k)^2 + \sum_{k=1}^{K-1} \rho(\theta_{k+1} - \theta_k). \]

We first claim that \( \hat{\theta}_k \in [\hat{Y}_1, \hat{Y}_K] \) for \( k = 1, \ldots, K \). To see this, suppose that this is not the case and define \( \hat{\theta} \) by projecting \( \theta \) onto \([\hat{Y}_1, \hat{Y}_K]^K \) (i.e. \( \hat{\theta}_k = \hat{Y}_K \wedge (\hat{Y}_1 \vee \theta_k) \) for \( k = 1, \ldots, K \)). The penalty contribution from \( \hat{\theta} \) is no larger than that of \( \theta \), and the loss contribution is strictly smaller, so we obtain the contradiction \( Q(\hat{\theta}) < Q(\theta) \).

We now proceed to show that for \( j = 1, \ldots, s-1 \), we have \( \hat{\theta}_{k_j} \leq \hat{Y}_{k_j} \) and \( \hat{\theta}_{k_{j+1}} \geq \hat{Y}_{k_j} \). We prove the first of these sets of inequalities, since the second follows similarly by considering the problem with \( -\hat{\theta}, -\hat{Y} \) and reversing the indices. Suppose, for contradiction, that there exists some \( j \) in \( \{1, \ldots, s-1\} \) with \( \hat{\theta}_{k_j} > \hat{Y}_{k_j} \). Let this \( j \) be minimal, such that for all \( l < j \) we have \( \hat{\theta}_{k_l} \leq \hat{Y}_{k_l} \).

Next define \( l_1 \) to be the maximal element of \( \{k_{j-1} + 1, \ldots, k_j - 1\} \) such that \( \hat{\theta}_{l_1} \leq \hat{Y}_{k_j} \). Similarly, we define \( l_2 \) to be minimal such that \( \hat{\theta}_{l_2} \geq \hat{Y}_{k_j} \). The existence of \( l_1 \) and \( l_2 \) is guaranteed by Lemma 8.

We note that for \( l = l_1 + 1, \ldots, k_j, \theta_l = \hat{\theta}_{k_j} \) and hence \( (\hat{Y}_l - \hat{\theta}_l)^2 \geq (\hat{Y}_{k_j} - \hat{\theta}_l)^2 = (\hat{Y}_{k_j} - \hat{\theta}_{k_j})^2 \). This can be shown by contradiction, as in (41). For such \( l \), we have from optimality of \( \hat{\theta} \) that \( \hat{Y}_l - \hat{\theta}_l \geq \hat{\theta}_{k_j} - \hat{Y}_l \) which implies that \( \theta_{l_1} < \hat{Y}_l \). From this it follows that \( (\hat{Y}_l - \hat{\theta}_l)^2 \leq \)
\((\hat{Y}_{k_j} - \hat{\theta}_{l_1})^2\). For such \(l\), it follows from the maximality of \(l_1\) that \(\hat{\theta}_{l_1} < \hat{Y}_l \leq \hat{Y}_{k_j}\) and therefore that \((\hat{Y}_l - \hat{\theta}_{l_1})^2 \leq (\hat{Y}_{k_j} - \hat{\theta}_{l_1})^2\).

Similarly, if \(l_2 > k_j + 1\), then for \(l = k_j + 1, \ldots, l_2 - 1\) we have \(\hat{\theta}_l = \hat{\theta}_{k_j+1}\) and hence \((\hat{Y}_l - \hat{\theta}_l)^2 \geq (\hat{Y}_{k_j+1} - \hat{\theta}_l)^2 = (\hat{Y}_{k_j+1} - \hat{\theta}_{k_j+1})^2\). For such \(l\), it follows that \(\hat{\theta}_{l_2} > \hat{Y}_l\) and therefore that \((\hat{Y}_l - \hat{\theta}_{l_2})^2 \leq (\hat{Y}_{k_j+1} - \hat{\theta}_{l_2})^2\).

Now, we define

\[
\tilde{w}_{k_j} := \sum_{l: \hat{\theta}_l = \hat{\theta}_{k_j}} w_l
\]

and, if \(l_2 > k_j + 1\),

\[
\tilde{w}_{k_j+1} := \sum_{l: \hat{\theta}_l = \hat{\theta}_{k_j+1}} w_l.
\]

We also define \(\tilde{\theta} \in \mathbb{R}^K\) according to

\[
\tilde{\theta}_l = \begin{cases} 
\hat{\theta}_l \land \hat{\theta}_{l_1} & \text{for } l \leq k_j \\
\hat{\theta}_l \lor \hat{\theta}_{l_2} & \text{for } l > k_j.
\end{cases}
\]

We note that by assumption, both \(\tilde{w}_{k_j} < 1/\eta_s\) and \(\tilde{w}_{k_j+1} < 1/\eta_s\). We now consider two cases: (A) where \(l_2 = k_j + 1\), so \(\hat{\theta}_{k_j+1} \geq \hat{Y}_{k_j+1}\), and (B) where \(l_2 > k_j + 1\), so \(\hat{\theta}_{k_j+1} < \hat{Y}_{k_j+1}\).

We first consider case (A), where the penalty terms between \(l_1\) and \(l_2\) in \(Q(\hat{\theta})\) are

\[
\sum_{l=1}^{l_2-1} \rho(\hat{\theta}_{l+1} - \hat{\theta}_l) = \rho(\hat{\theta}_{l_2} - \hat{\theta}_{k_j}) + \rho(\hat{\theta}_{k_j} - \hat{\theta}_{l_1}).
\]

Thus,

\[
Q(\hat{\theta}) - Q(\tilde{\theta}) \geq \frac{\tilde{w}_{k_j}}{2}(\hat{Y}_{k_j} - \hat{\theta}_{k_j})^2 - \frac{\tilde{w}_{k_j}}{2}(\hat{Y}_{k_j} - \hat{\theta}_{l_1})^2 + \frac{\tilde{w}_{k_j}}{2}(\hat{Y}_{k_j} - \hat{\theta}_{l_1})^2
\]

\[
+ \rho(\hat{\theta}_{l_2} - \hat{\theta}_{k_j}) + \rho(\hat{\theta}_{k_j} - \hat{\theta}_{l_1}) - \frac{1}{2} \gamma \lambda^2
\]

\[
\geq \inf_{\hat{Y}_{k_j} < a < \hat{Y}_{k_j+1}} \frac{\tilde{w}_{k_j}}{2}(\hat{Y}_{k_j} - a)^2 - \frac{\tilde{w}_{k_j}}{2}(\hat{Y}_{k_j} - \hat{\theta}_{l_1})^2
\]

\[
+ \rho(\hat{\theta}_{l_2} - a) + \rho(a - \hat{\theta}_{l_1}) - \frac{1}{2} \gamma \lambda^2.
\]

We specify the infimum in (33) because \((\hat{Y}_{k_j}, \hat{Y}_{k_j+1})\) is not closed, and let \((a_m)\) be a convergent sequence in \((\hat{Y}_{k_j}, \hat{Y}_{k_j+1})\) whose limit attains this infimum. We define \(a^* = \lim_{m \to \infty} a_m\).

By assumption (29), at least one of \((a^* - \hat{\theta}_{l_1})\) and \((\hat{\theta}_{l_2} - a^*)\) is greater than or equal to \(\gamma \lambda\). Here, we use that the separation (29) \(\geq 2\gamma \lambda\). If \(\hat{\theta}_{l_2} - a^* \geq \gamma \lambda\) then we denote this case (A1) and (31) becomes

\[
Q(\hat{\theta}) - Q(\tilde{\theta}) \geq \inf_{\hat{Y}_{k_j} < a < \hat{\theta}_{l_2} - \gamma \lambda} \frac{\tilde{w}_{k_j}}{2}(\hat{Y}_{k_j} - a)^2 - \frac{\tilde{w}_{k_j}}{2}(\hat{Y}_{k_j} - \hat{\theta}_{l_1})^2 + \rho(a - \hat{\theta}_{l_1})
\]

\[
\geq \min_{\hat{\theta}_{l_1} \leq a \leq \hat{\theta}_{l_2} - \gamma \lambda} \frac{\tilde{w}_{k_j}}{2}(\hat{Y}_{k_j} - a)^2 - \frac{\tilde{w}_{k_j}}{2}(\hat{Y}_{k_j} - \hat{\theta}_{l_1})^2 + \rho(\hat{a} - \hat{\theta}_{l_1}).
\]

We define \(\bar{a}^*\) to be the minimiser over \(\hat{a}\) of (33). We can observe that since \(\hat{Y}_{k_j} - \hat{\theta}_{l_1} < \zeta\) and \(\zeta < (1 \land \sqrt{\gamma \tilde{w}_{k_j}}) \lambda / \tilde{w}_{k_j}\), we have \(\hat{Y}_{k_j} - \hat{\theta}_{l_1} < (1 \land \sqrt{\gamma \tilde{w}_{k_j}}) \lambda / \tilde{w}_{k_j}\). Thus, we have by Lemma 6 that the uniquely optimal \(\bar{a}^* = \hat{\theta}_{l_1}\). This gives that the value of (33) is zero.
It is straightforward to see from (32) that $a^* = \hat{Y}_{k_j}$ must be the unique limit of $(a_m)$. As we have assumed that $\hat{\theta}_{k_j} > \hat{Y}_{k_j}$ and the infimum is not attained in $(\hat{Y}_{k_j}, \hat{Y}_{k_j+1})$, the inequality in line (32) can be made strict. It follows that $Q(\hat{\theta}) > Q(\hat{\theta})$.

Thus, it remains for us to consider the case where $\hat{\theta}_{l_2} - a^* < \gamma \lambda$, which implies that $a^* - \hat{\theta}_{l_1} \geq \gamma \lambda$. We denote this case (A2). Now, from (31) we can obtain

$$Q(\hat{\theta}) - Q(\hat{\theta}) \geq \frac{\tilde{w}_{k_j}}{2} (\hat{Y}_{k_j} - \hat{\theta}_{l_2} - \hat{\theta}_{l_1})^2 - \frac{\tilde{w}_{k_j}}{2} (\hat{Y}_{k_j} - \hat{\theta}_{l_2})^2 = \rho(\hat{\theta}_{l_2} - \hat{\theta}_{l_1}).$$

(34)

The objective of this function is piecewise quadratic (and continuously differentiable), with two pieces: $[\hat{\theta}_{l_1}, \hat{\theta}_{l_2} - \gamma \lambda]$ and $(\hat{\theta}_{l_2} - \gamma \lambda, \hat{\theta}_{l_2})$. On the first region, the objective is a convex quadratic with minimum at $\hat{Y}_{k_j} \in [\hat{\theta}_{l_1}, \hat{\theta}_{l_2} - \gamma \lambda]$.

By the assumption that $a^* \geq \hat{\theta}_{l_2} - \gamma \lambda$, we know that the objective must be concave on $[\hat{\theta}_{l_2} - \gamma \lambda, \hat{\theta}_{l_2}]$. It is clear that the derivative of the objective at $\hat{\theta}_{l_2} - \gamma \lambda$ is positive. Hence, if $\tilde{a}^* = \hat{\theta}_{l_2} - \gamma \lambda$, then the objective will take a strictly lower value at some $\tilde{a}^* \in (\hat{\theta}_{l_2} - \gamma \lambda, \hat{\theta}_{l_2})$ (for some small $\epsilon > 0$), contradicting optimality of $\tilde{a}^*$. It therefore follows that $\tilde{a}^* = \hat{\theta}_{l_2}$.

With this knowledge, we can further simplify (34) to obtain

$$Q(\hat{\theta}) - Q(\hat{\theta}) \geq \frac{\tilde{w}_{k_j}}{2} (\hat{Y}_{k_j} - \hat{\theta}_{l_2})^2 - \frac{\tilde{w}_{k_j}}{2} (\hat{Y}_{k_j} - \hat{\theta}_{l_1})^2 > 0.$$  

The second inequality follows from $\hat{Y}_{k_j} - \hat{\theta}_{l_1} \leq \zeta$ and $\hat{\theta}_{l_2} - \hat{Y}_{k_j} > \zeta$. Hence, we obtain that $Q(\hat{\theta}) > Q(\hat{\theta})$.

We now direct our attention towards case (B), where similarly to before we observe that the penalty contributions between $l_1$ and $l_2$ in $Q(\hat{\theta})$ are

$$\sum_{l_2-1}^{l_2-1} \rho(\hat{\theta}_{l_1} - \hat{\theta}_l) = \rho(\hat{\theta}_{l_1} - \hat{\theta}_{l_1+1}) + \rho(\hat{\theta}_{l_1+1} - \hat{\theta}_{l_1}) + \rho(\hat{\theta}_{k_j+1} - \hat{\theta}_{l_1}).$$

As for case (A), we obtain

$$Q(\hat{\theta}) - Q(\hat{\theta}) \geq \frac{\tilde{w}_{k_j}}{2} (\hat{Y}_{k_j} - \hat{\theta}_{l_2})^2 - \frac{\tilde{w}_{k_j}}{2} (\hat{Y}_{k_j} - \hat{\theta}_{k_j+1})^2 - \frac{\tilde{w}_{k_j}}{2} (\hat{Y}_{k_j} - \hat{\theta}_{l_1})^2 - \frac{\tilde{w}_{k_j}}{2} (\hat{Y}_{k_j} - \hat{\theta}_{l_2})^2 \geq \frac{\tilde{w}_{k_j}}{2} (\hat{Y}_{k_j} - a)^2 + \frac{\tilde{w}_{k_j+1}}{2} (\hat{Y}_{k_j+1} - b)^2 \geq \frac{\tilde{w}_{k_j}}{2} (\hat{Y}_{k_j} - a)^2 + \frac{\tilde{w}_{k_j+1}}{2} (\hat{Y}_{k_j+1} - b)^2 - \frac{\tilde{w}_{k_j}}{2} (\hat{Y}_{k_j} - \hat{\theta}_{l_1})^2 - \frac{\tilde{w}_{k_j}}{2} (\hat{Y}_{k_j} - \hat{\theta}_{l_2})^2 + \rho(\hat{\theta}_{l_2} - b) + \rho(b - a) + \rho(a - \hat{\theta}_{l_1}) + \frac{1}{2} \gamma \lambda^2.$$  

(35)

We specify the infimum in (36) because $(\hat{Y}_{k_j}, \hat{Y}_{k_j+1})$ is not closed and therefore a minimum may not exist. Let $(a_m, b_m)$ be a convergent sequence in $(\hat{Y}_{k_j}, \hat{Y}_{k_j+1})$ whose limit achieves this infimum. We now define $(a^*, b^*) = \lim_{m \to \infty} (a_m, b_m)$. By assumption (29), we know that $\hat{Y}_{k_j+1} - \hat{Y}_{k_j} \geq 3 \gamma \lambda$, which implies that $\hat{\theta}_{l_2} - \hat{\theta}_{l_1} \geq 3 \gamma \lambda$. Thus, one of $\{(\hat{\theta}_{l_2} - b^*), (b^* - a^*), (a^* - \hat{\theta}_{l_1})\}$ must be at least $\gamma \lambda$. 

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We first consider if \( b^* - a^* \geq \gamma \lambda \), and denote this case (B1). Here, (36) becomes

\[
Q(\hat{\theta}) - Q(\hat{\theta}) \geq \inf_{\tilde{b} \leq b < Y_{k_j+1}} \frac{\tilde{w}_{k_j}}{2}(Y_{k_j} - \tilde{a})^2 + \frac{\tilde{w}_{k_j+1}}{2}(Y_{k_j+1} - \tilde{b})^2 - \frac{\tilde{w}_{k_j}}{2}(Y_{k_j} - \hat{\theta}_1)^2 - \frac{\tilde{w}_{k_j+1}}{2}(Y_{k_j+1} - \hat{\theta}_2)^2 + \rho(\hat{\theta}_2 - b) + \rho(a - \hat{\theta}_1)
\]

\[= \inf_{a \leq b \leq Y_{k_j+1}} \left\{ \frac{\tilde{w}_{k_j}}{2}(Y_{k_j} - \tilde{a})^2 - \frac{\tilde{w}_{k_j}}{2}(Y_{k_j} - \hat{\theta}_1)^2 \right\} + \inf_{b \in (Y_{k_j}, Y_{k_j+1})} \left\{ \frac{\tilde{w}_{k_j+1}}{2}(Y_{k_j+1} - \tilde{b})^2 - \frac{\tilde{w}_{k_j+1}}{2}(Y_{k_j+1} - \hat{\theta}_2)^2 + \rho(\hat{\theta}_2 - b) \right\}
\]

(37)

We can observe that (38) is the sum of two copies of (32) in case (A1). Hence, by following the same arguments as before, we see that \( Q(\hat{\theta}) > Q(\hat{\theta}) \).

It therefore remains for us to obtain the result in the case that \( b^* - a^* < \gamma \lambda \), and we denote this case (B2). Using that the separation (29) \( \geq 3\gamma \lambda + 2\zeta \), it is straightforward to see that one of \((Y_{k_j+1} - b^*)\) and \((a^* - Y_{k_j})\) must be at least \( \gamma \lambda + \zeta \). By the symmetry of the problem, it is sufficient for us to consider the case where \( Y_{k_j+1} - b^* \geq \gamma \lambda + \zeta \). In this case, we can obtain from (36) that

\[
Q(\hat{\theta}) - Q(\hat{\theta}) \geq \min_{(\tilde{a}, \tilde{b}) \in B} \left\{ \frac{\tilde{w}_{k_j}}{2}(Y_{k_j} - \tilde{a})^2 + \frac{\tilde{w}_{k_j+1}}{2}(Y_{k_j+1} - \tilde{b})^2 - \frac{\tilde{w}_{k_j}}{2}(Y_{k_j} - \hat{\theta}_1)^2 - \frac{\tilde{w}_{k_j+1}}{2}(Y_{k_j+1} - \hat{\theta}_2)^2 + \rho(\hat{\theta}_2 - \tilde{b}) + \rho(\tilde{a} - \hat{\theta}_1) \right\}
\]

where \( B = \{(\tilde{a}, \tilde{b}) : \hat{\theta}_1 \leq \tilde{a} \leq \tilde{b} \leq Y_{k_j+1} - \gamma \lambda - \zeta, \tilde{b} - \tilde{a} < \gamma \lambda \} \). From this, we can extract the terms dependent on \( \tilde{b} \) to obtain

\[
\tilde{b}^* = \arg \min_{\tilde{a}^* \leq \tilde{b} < \tilde{a}^* + \gamma \lambda} \frac{\tilde{w}_{k_j+1}}{2}(Y_{k_j+1} - \tilde{b})^2 + \rho(\tilde{b} - \tilde{a}^*).
\]

(40)

The objective of this function is piecewise quadratic (and continuously differentiable), with two pieces: \([\tilde{a}^*, \tilde{a}^* + \gamma \lambda]\) and \([\tilde{a}^* + \gamma \lambda, \hat{\theta}_2]\). Over the second region, the objective is a convex quadratic with minimum at \( Y_{k_j+1} \in [\tilde{a}^* + \gamma \lambda, \hat{\theta}_2] \). By following the same argument as for (34) in case (A2), we see that \( \tilde{b}^* = \tilde{a}^* \).

With this knowledge, we can further simplify (39) to obtain

\[
Q(\hat{\theta}) - Q(\hat{\theta}) \geq \min_{\hat{\theta}_1 \leq \tilde{a} \leq Y_{k_j+1} - \gamma \lambda - \zeta} \left\{ \frac{\tilde{w}_{k_j}}{2}(Y_{k_j} - \tilde{a})^2 + \frac{\tilde{w}_{k_j+1}}{2}(Y_{k_j+1} - \tilde{a})^2 - \frac{\tilde{w}_{k_j}}{2}(Y_{k_j} - \hat{\theta}_1)^2 - \frac{\tilde{w}_{k_j+1}}{2}(Y_{k_j+1} - \hat{\theta}_2)^2 + \rho(\tilde{a} - \hat{\theta}_1) \right\}.
\]

Since \( Y_{k_j+1} - \tilde{a}^* > \zeta \), we can see that \((Y_{k_j+1} - \tilde{a}^*)^2 - (Y_{k_j+1} - \hat{\theta}_2)^2 > 0 \). Thus, it suffices for us to show that

\[
\min_{\hat{\theta}_1 \leq \tilde{a} \leq Y_{k_j+1} - \gamma \lambda - \zeta} \left\{ \frac{\tilde{w}_{k_j}}{2}(Y_{k_j} - \tilde{a})^2 - \frac{\tilde{w}_{k_j}}{2}(Y_{k_j} - \hat{\theta}_1)^2 + \rho(\tilde{a} - \hat{\theta}_1) \right\} \geq 0.
\]
This objective is exactly as in (33) in case (A1), minimised over a smaller feasible set. Hence, it follows immediately that this holds and we can conclude that \( Q(\hat{\theta}) > Q(\tilde{\theta}) \).

We now have for all cases that \( Q(\theta) > Q(\hat{\theta}) \), which contradicts the optimality of \( \hat{\theta} \). Thus, we can conclude that for \( j = 1, \ldots, s \), \( \hat{\theta}_{k_j} \leq \tilde{Y}_{k_j} \) and \( \hat{\theta}_{k_j+1} \geq \tilde{Y}_{k_j+1} \).

\[ \Box \]

Lemma 8. Consider the setup of Lemma 7. For each \( j = 1, \ldots, s \), there exists \( k^*_j \) in \( \{k_{j-1} + 1, \ldots, k_j\} \) such that \( \hat{\theta}_{k^*_j} \in [\tilde{Y}_{k_{j-1}+1}, \tilde{Y}_{k_j}] \).

Proof. We first show that if \( \hat{\theta}_{k_j} > \tilde{Y}_{k_j}, \) then for any \( k \) with \( k_{j-1} + 1 \leq k \leq k_j \), if \( \hat{\theta}_k > \tilde{Y}_{k_j} \) then \( \hat{\theta}_k = \hat{\theta}_{k_j} \).

We prove the first case since the proof for the second is identical. Suppose that this does not hold, i.e., \( \hat{\theta}_{k_j} > \tilde{Y}_{k_j} \) and there exists some (minimal) \( k \) in \( \{k_{j-1} + 1, \ldots, k_j - 1\} \) with \( \tilde{Y}_{k_j} < \hat{\theta}_k < \hat{\theta}_{k_j} \). Then we construct \( \tilde{\theta} \) by

\[
\tilde{\theta}_l = \begin{cases} 
\hat{\theta}_k & \text{for } l = k, k+1, \ldots, k_j \\
\hat{\theta}_l & \text{otherwise.}
\end{cases}
\] (41)

We observe that the penalty contribution from \( \hat{\theta} \) is no more than that of \( \tilde{\theta} \) and that the quadratic loss for \( \tilde{\theta} \) will be strictly less than that of \( \hat{\theta} \). This gives us that \( Q(\tilde{\theta}) < Q(\hat{\theta}) \), contradicting the optimality of \( \hat{\theta} \).

Similarly, if \( \hat{\theta}_{k_{j-1}+1} < \tilde{Y}_{k_{j-1}+1} \) then the corresponding statement that for any \( k \) with \( k_{j-1} + 1 \leq k \), if \( \hat{\theta}_k < \tilde{Y}_{k_{j-1}+1} \) then \( \hat{\theta}_k = \hat{\theta}_{k_{j-1}+1} \).

We now establish a simple preliminary result. Suppose that for some \( j \) in \( \{1, \ldots, s\} \) there exists \( k \) in \( \{k_{j-1} + 1, \ldots, k_j\} \) with \( \hat{\theta}_k \notin [\tilde{Y}_{k_{j-1}+1}, \tilde{Y}_{k_j}] \), such that \( \sum_{l: \hat{\theta}_l = \hat{\theta}_k} w_l \geq \eta/2s \). We claim that if \( \hat{\theta}_k > \tilde{Y}_{k_j} \) then \( \hat{\theta}_k \leq \tilde{Y}_{k_j} + (\sqrt{2s/\eta} \sqrt{\gamma \lambda} \vee \gamma \lambda) \). Similarly, if \( \hat{\theta}_k < \tilde{Y}_{k_{j-1}+1} \) then \( \hat{\theta}_k \geq \tilde{Y}_{k_{j-1}+1} - (\sqrt{2s/\eta} \sqrt{\gamma \lambda} \vee \gamma \lambda) \).

To prove the claim, we consider the case \( \hat{\theta}_k > \tilde{Y}_{k_j} \) (the other is identical). By the first observation, if \( \hat{\theta}_l > \tilde{Y}_{k_j} \) for \( l \) in \( \{k_{j-1} + 1, \ldots, k_j\} \) then \( \hat{\theta}_l = \hat{\theta}_k \). Now, for contradiction, suppose \( \hat{\theta}_k > \tilde{Y}_{k_j} + (\sqrt{2s/\eta} \sqrt{\gamma \lambda} \vee \gamma \lambda) \) and let this \( k \) be minimal. Then we can construct \( \tilde{\theta} \) by

\[
\tilde{\theta}_l = \begin{cases} 
\sum_{l=k}^{k_j} w_l \tilde{Y}_l/\sum_{l=k}^{k_j} w_l & \text{for } l = k, \ldots, k_j \\
\hat{\theta}_l & \text{otherwise.}
\end{cases}
\]

By appealing to the optimality of \( \hat{\theta} \), we can easily observe that \( \hat{\theta}_{k-1} \leq \tilde{Y}_{k-1} \) and therefore that the ordering of the entries of \( \tilde{\theta} \) matches that of \( \hat{\theta} \). Here, we use that \( (\sqrt{2s/\eta} \sqrt{\gamma \lambda} \vee \gamma \lambda) \geq \gamma \lambda \).

We can now see that the loss term in \( Q(\tilde{\theta}) \) is less than in \( Q(\hat{\theta}) \), with a difference of more than \( (\eta/4s)(\sqrt{2s/\eta} \sqrt{\gamma \lambda})^2 \) = \( \gamma \lambda^2 / 2 \), which outweighs the possible increase in the penalty contribution.

This gives us that \( Q(\tilde{\theta}) < Q(\hat{\theta}) \), contradicting the optimality of \( \hat{\theta} \).

We now return to the proof of the main result. Suppose, for contradiction, that there exists some \( j \) in \( \{1, \ldots, s\} \) such that \( \hat{\theta}_k \notin [\tilde{Y}_{k_{j-1}+1}, \tilde{Y}_{k_j}] \) for all \( k = k_{j-1} + 1, \ldots, k_j \) and let this \( j \) be minimal. By the first observation, we know that entries of \( \hat{\theta} \) corresponding to level \( j \) can take one of at most two distinct values. That is, for \( k \in \{k_{j-1} + 1, \ldots, k_j\} \), if we have \( \hat{\theta}_k < \tilde{Y}_{k_{j-1}+1} \), then it follows that \( \hat{\theta}_k = \hat{\theta}_{k_{j-1}+1} \). Similarly, if \( \hat{\theta}_k > \tilde{Y}_{k_j} \), then \( \hat{\theta}_k = \hat{\theta}_{k_j} \).

By the assumption \( w_{\min} \geq \eta/s \), we have that either

\[
\sum_{k: \hat{\theta}_k = \hat{\theta}_{k_{j-1}+1}} w_k \geq \frac{\eta}{2s} \quad \text{or} \quad \sum_{k: \hat{\theta}_k = \hat{\theta}_{k_j}} w_k \geq \frac{\eta}{2s}.
\]
We will without loss of generality take the second statement to be true (the proof for the first case follows identically). Let $k'$ denote the minimal element in \{\(k_{j-1} + 1, \ldots, k_j\)\} such that \(\hat{\theta}_{k'} = \hat{\theta}_{k_j}\). From the preliminary result established earlier, \(\hat{\theta}_{k_j} \leq \bar{Y}_{k_j} + (\sqrt{2s/\eta} \sqrt{\gamma \lambda} + \gamma \lambda)\). By appealing to the optimality of \(\hat{\theta}\), we see that \(\hat{\theta}_{k_j+1} < \hat{\theta}_{k_j} + \gamma \lambda\) (otherwise, we could take \(\hat{\theta}_{k_j}\) to be \(\bar{Y}_{k_j}\) and strictly reduce the value of the objective). Here, we use that the separation is at least \(2(\sqrt{2s/\eta} \sqrt{\gamma \lambda} + \gamma \lambda)\).

By our earlier observation, it is clear that any \(l \in \{k_j + 1, \ldots, k_{j+1}\}\) with \(\hat{\theta}_l < \bar{Y}_{k_{j+1}}\) has \(\hat{\theta}_l = \hat{\theta}_{k_{j+1}}\). Note that since \(\hat{\theta}_{k_{j+1}} - \bar{Y}_{k_j} < (\sqrt{2s/\eta} \sqrt{\gamma \lambda} \lor \gamma \lambda)\), it follows that \(\bar{Y}_{k_{j+1}} - \hat{\theta}_{k_{j+1}} > (\sqrt{2s/\eta} \sqrt{\gamma \lambda} \lor \gamma \lambda) + \zeta\) and therefore that \(\sum_{\{k: \hat{\theta}_k = \hat{\theta}_{k_{j+1}}\}} \gamma \lambda < \eta / 2s\) by the preliminary result. Since \(w_{\min}^0 < \eta / s\) and separation (29) \(\geq 2(\sqrt{2s/\eta} \sqrt{\gamma \lambda} \lor \gamma \lambda) + \gamma \lambda + \zeta\), we can define \(l' \in \{k_j + 1, \ldots, k_{j+1}\}\) minimal such that \(\hat{\theta}_{l'} \geq \bar{Y}_{k_{j+1}}\).

Now, in order to contradict the optimality of \(\hat{\theta}\) we construct a new feasible point \(\bar{\theta}\) by setting

\[
\bar{\theta}_l = \begin{cases} \bar{Y}_{k_j} & \text{for } l = k', \ldots, k_j \\ \hat{\theta}_{l'} & \text{for } l = k_j + 1, \ldots, l' - 1 \\ \hat{\theta}_l & \text{otherwise.} \end{cases}
\]

It follows that for \(l = k_j + 1, \ldots, l' - 1\) we have

\[
|\hat{\theta}_l - \bar{Y}_l| > (\sqrt{2s/\eta} \sqrt{\gamma \lambda} \lor \gamma \lambda) + \zeta
\]

\[
|\hat{\theta}_l - \bar{Y}_l| \leq (\sqrt{2s/\eta} \sqrt{\gamma \lambda} \lor \gamma \lambda) + \zeta.
\]

It is also straightforward to see that \(|\hat{\theta}_{k_j} - \bar{Y}_{k_j}| \geq |\bar{Y}_{k_{j+1}} - \bar{Y}_l|\) for \(l = k', \ldots, k_j\). If follows that the loss contribution in \(Q(\hat{\theta})\) is strictly less than that in \(Q(\bar{\theta})\). Hence, using \(\hat{\theta}_{l'} - \hat{\theta}_{k_j} > \gamma \lambda\), we obtain

\[
Q(\hat{\theta}) - Q(\bar{\theta}) > \rho(\hat{\theta}_{l'} - \hat{\theta}_{k_{j+1}}) + \rho(\hat{\theta}_{k_{j+1}} - \hat{\theta}_{k_j}) + \rho(\hat{\theta}_{k_j} - \hat{\theta}_{k'-1})
\]

\[
- \frac{1}{2} \gamma \lambda^2 - \rho(\bar{Y}_{k_j} - \hat{\theta}_{k'-1})
\]

\[
\geq 0,
\]

contradicting the optimality of \(\hat{\theta}\). We conclude that for \(j = 1, \ldots, s\), there exists \(k_j^*\) in \(\{k_{j-1} + 1, \ldots, k_j\}\) such that \(\hat{\theta}_j^* \in [\bar{Y}_{k_{j-1}+1}, \bar{Y}_{k_j}]\).

**Lemma 9.** Consider the univariate objective (10), relaxing the normalisation constraint to \(\bar{w} := \sum_k w_k \leq 1\). Suppose that \(w\bar{Y} = 0\), and that \(\|\bar{Y}\|_\infty < (2 \land \sqrt{\gamma / w}) \lambda / \bar{w}\). Then \(\hat{\theta} = 0\).

**Proof.** Let \(P_w = I - 1w^T / \bar{w}\) and \(D_w \in \mathbb{R}^{K \times K}\) be the diagonal matrix with entries \(D_{kk} \sqrt{w_k}\). First note that

\[
Q(\theta) - Q(P_w \theta) = \frac{1}{2} \sum_{k=1}^{K} w_k (\bar{Y}_k - \theta_k)^2 - \frac{1}{2} \sum_{k=1}^{K} w_k (\bar{Y}_k - \theta_k + w^T \theta)^2
\]

\[
= -\frac{1}{2} \sum_{k=1}^{K} w_k (w^T \theta) (2\bar{Y}_k - 2\theta_k + w^T \theta)
\]

\[
= \left(1 - \frac{1}{2} \bar{w}\right) (w^T \theta)^2 \geq 0.
\]
Thus for all $\theta \in \mathbb{R}^K$, we have
\[
Q(\theta) - Q(0) \geq \frac{1}{2} \| D_w P_w (\tilde{Y} - \theta) \|_2^2 - \frac{1}{2} \| D_w P_w \tilde{Y} \|_2^2 + \sum_{k=1}^{K-1} \rho(\theta_{(k+1)} - \theta_{(k)}) \\
\geq \frac{1}{2} \| D_w P_w (\tilde{Y} - \theta) \|_2^2 - \frac{1}{2} \| D_w P_w \tilde{Y} \|_2^2 + \rho(\theta_{(K)} - \theta_{(1)}) \\
\geq \min_{\xi \in [-\tau, \tau]^K} F(\theta, \xi, w)
\]
where
\[
F(\theta, \xi, w) = \frac{1}{2} \| D_w P_w (\xi - \theta) \|_2^2 - \frac{1}{2} \| D_w P_w \xi \|_2^2 + \rho(\theta_{(K)} - \theta_{(1)}).
\]

Consider minimising $F$ over $\mathbb{R}^K \times [-\tau, \tau]^K \times S$, where $S \subseteq \mathbb{R}^K$ is the unit simplex scaled by $\tilde{w}$. We aim to show this minimum is 0. As with the first claim in the proof of Lemma 7, it is straightforward to see that for any feasible $(\theta, \xi, w)$, there exists $\theta'$ with $\|\theta'\|_\infty \leq \|\xi\|_\infty$ and $F(\theta', \xi, w) \leq F(\theta, \xi, w)$. Hence,
\[
\inf_{(\theta, \xi, w) \in \mathbb{R}^K \times [-\tau, \tau]^K \times S} F(\theta, \xi, w) = \inf_{(\theta, \xi, w) \in [-\tau, \tau]^K \times [-\tau, \tau]^K \times S} F(\theta, \xi, w).
\]
As on the RHS we are minimising a continuous function over a compact set, we know a minimiser must exist. Let $(\tilde{\theta}, \tilde{\xi}, \tilde{w})$ be a minimiser (to be specified later). Observe that
\[
\| D_w P_w (\xi - \theta) \|_2^2 - \| D_w P_w \xi \|_2^2 = -2\xi^T P_w^T D_w^2 P_w \theta + \tilde{\theta}^T P_w^T D_w^2 P_w \theta
\]
is linear as a function of $\xi$. Hence it is minimised over the set
\[
\{ \xi : \|\xi\|_\infty \leq \tau \} = \text{conv}(\{-\tau, \tau\}^K)
\]
at some point in $\{-\tau, \tau\}^K$. Here $\text{conv}(\cdot)$ denotes the convex hull operation. We thus have
\[
Q(\theta) - Q(0) \geq \min_{\xi \in [-\tau, \tau]^K} \frac{1}{2} \| D_w P_w (\xi - \theta) \|_2^2 - \frac{1}{2} \| D_w P_w \xi \|_2^2 + \rho(\theta_{(K)} - \theta_{(1)}).
\]
Let us take $(\tilde{\theta}, \tilde{\xi}) \in \mathbb{R}^K \times [-\tau, \tau]^K$ to be a minimiser of the RHS.

Note that if we have $\tilde{\xi}_j = \xi_k$ then we may take $\tilde{\theta}_j = \hat{\theta}_k$. Indeed, we may construct $\tilde{\theta} \in \mathbb{R}^K$ by setting
\[
\tilde{\theta}_l = \begin{cases} \arg \min_{b \in \{\hat{\theta}_j, \hat{\theta}_k\}} (\tilde{\xi}_j - b)^2 & \text{for } l = j, k \\ \hat{\theta}_l & \text{otherwise.} \end{cases}
\]
Since the penalty contribution from $\tilde{\theta}$ is not greater than that of $\hat{\theta}$, it follows that $Q(\tilde{\theta}) \leq Q(\hat{\theta})$. Thus, we can assume that entries of $\tilde{\theta}$ can take one of only two distinct values.

Next we write $\tilde{\alpha} = \sum_{k, \xi_k = -\tau} \tilde{w}_k$ and observe that $\tilde{w}^T \tilde{\xi} = (\tilde{w} - 2\tilde{\alpha})\tau$. Let us set $s = \min_k \tilde{\theta}_k$ and $x = \max_k \tilde{\theta}_k - \min_k \tilde{\theta}_k$. Then we have
\[
F(\tilde{\theta}, \tilde{\xi}, \tilde{w}) = \frac{1}{2} \tilde{\alpha}((2\tilde{\alpha} - 1 - \tilde{w})\tau - s)^2 + \frac{1}{2}(\tilde{w} - \tilde{\alpha})((2\tilde{\alpha} + 1 - \tilde{w})\tau - s - x)^2 \\
+ \rho(x) - \frac{2}{\tilde{w}}\tilde{\alpha}(\tilde{w} - \tilde{\alpha})\tau^2 \\
= \frac{1}{2\tilde{w}}\tilde{\alpha}(\tilde{w} - \tilde{\alpha})(2\tau - x)^2 + \rho(x) - \frac{2}{\tilde{w}}\tilde{\alpha}(\tilde{w} - \tilde{\alpha})\tau^2 \\
= \frac{\tilde{w}}{8}(2\tau - x)^2 + \rho(x) - \frac{1}{2} \tau^2.
\]

(42)
In the second line above, we have solved for \( s \) to find that
\[
s = \frac{1}{\hat{w}} \left\{ \tau (1 - \hat{w}) (\hat{w} - 2\hat{\alpha}) + (\hat{\alpha} - \hat{w}) \right\}.
\]
In the third line above, we have solved for \( \hat{\alpha} \) to obtain \( \hat{\alpha} = \hat{w}/2 \) and hence \( \hat{\alpha}(\hat{w} - \hat{\alpha})/\hat{w} = \hat{w}/4 \). These follow from optimality of \( \hat{\theta} \) and \( \hat{w} \) respectively. The result follows from applying Lemma 6, setting \( \kappa = \hat{w}/4 \).

### S3.3 Proof of Theorem 5

Define \( P^0 \) to be the orthogonal projection onto the linear space \( \Theta_0 \). The residuals from the oracle least squares fit are \( (I - P^0)\varepsilon \). Since the entries of \( \varepsilon \) are \( \sigma \)-sub-Gaussian, it follows that the entries of \( (I - P^0)\varepsilon \) are also \( \sigma \)-sub-Gaussian.

The partial residuals \( R^{(j)} \) as defined in (12) for the \( j \)th variable are therefore
\[
R^{(j)}_i = \sum_{k=1}^{K_j} \mathbb{1}_{\{X_{ij} = k\}} \hat{\theta}^{(j)}_{jk} + \left[ (I - P^0)\varepsilon \right]_i.
\]
Similarly to before, for \( k = 1, \ldots, K_j \), define \( \bar{R}^{(j)}_k = \sum_{i=1}^{n} \mathbb{1}_{\{X_{ij} = k\}} R^{(j)}_i / n_{jk} \). We aim to apply Theorem 4 to the univariate problem for each \( j \) to show that \( \hat{\theta}^0 \) is a fixed point of block coordinate descent (see Section 3.2), with the oracle least squares solution as the signal.

We directly apply the results of Theorem 5 to this univariate problem, noting that we require minimum separation (18),
\[
\Delta(\hat{\theta}^0_j) \geq 3 \left( 1 + \frac{\sqrt{2}}{\eta} \right) \sqrt{\gamma_j \gamma^*_j \lambda_j},
\]
We obtain this by working on the event \( \|\hat{\theta}^0_j - \theta^0_j\|_\infty \leq \tau_j \) and appealing to the triangle inequality with (20).

We must now bound the probability of the union of all these events occurring. First, we require a copy of (19) for each variable \( j \) that comes from applying Theorem 4 to each subproblem. Using a union bound, this occurs with probability at least
\[
1 - 2 \sum_{j=1}^{p} \exp \left( - \frac{n w_{j,\text{min}} \gamma_j \gamma^*_j \lambda_j^2}{8 \sigma^2} + \log(K_j) \right),
\]
where we use a sub-Gaussian tail bound on linear combinations of the \( \left[ (I - P^0)\varepsilon \right]_i \) (and recall that \( w_{jk} = n_{jk}/n \)). Secondly, for the signal variables (i.e. those \( j \) for which \( s_j > 1 \)), we must check that \( \|\theta^0 - \theta^0_j\|_\infty \leq \tau_j \). Using a union bound, this occurs with probability at least
\[
1 - 2 \sum_{j \in S} \exp \left( - \frac{n w^0_{j,\text{min}} \tau_j^2}{2 \sigma^2} + \log(s_j) \right).
\]
We now set \( \tau_j = \sqrt{\gamma_j \gamma^*_j \lambda_j} / 2 \) and observe that the separation bound becomes
\[
\Delta(\theta^0_j) \geq 2\tau_j + \Delta(\hat{\theta}^0_j) \geq 3 \left( 1 + \frac{\sqrt{2}}{\eta} \right) \sqrt{\gamma_j \gamma^*_j \lambda_j} + \sqrt{\gamma_j \gamma^*_j \lambda_j}.
\]
Using a final union bound to combine these expressions, we observe that \( s_j \leq K_j \) and \( w_{j,\text{min}} \leq w^0_{j,\text{min}} \), yielding the simplified bound (21).
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