

On b -bit min-wise hashing for large-scale regression and classification with sparse data

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April 30, 2016

Abstract

Large-scale regression problems where both the number of variables, p , and the number of observations, n , may be large and in the order of millions or more, are becoming increasingly more common. Typically the data are sparse: only a fraction of a percent of the entries in the design matrix are non-zero. Nevertheless, often the only computationally feasible approach is to perform dimension reduction to obtain a new design matrix with far fewer columns, and then work with this compressed data.

b -bit min-wise hashing [Li and König, 2011, Li et al., 2011] is a promising dimension reduction scheme for sparse matrices. In this work we study the prediction error of procedures which perform regression in the new lower-dimensional space after applying the method. For both linear and logistic models we show that the average prediction error vanishes asymptotically as long as $q\|\beta^*\|_2^2/n \rightarrow 0$, where q is the average number of non-zero entries in each row of the design matrix and β^* is the coefficient of the linear predictor.

We also show that ordinary least squares or ridge regression applied to the reduced data in a sense amounts to a non-parametric regression and can in fact allow us fit more flexible models. We obtain non-asymptotic prediction error bounds for interaction models and for models where an unknown row normalisation must be applied before the signal is linear in the predictors.

1 Introduction

The modern field of high-dimensional statistics has now developed a powerful range of methods to deal with datasets where the number of variables p may greatly exceed the number of variables n (see Bühlmann and van de Geer [2011] for an overview of recent advances). The prototypical example of microarray data, where p may be in the tens of thousands but n is typically not more than a few hundred, has motivated much of this development. Yet not all modern datasets come in this sort of shape and size. The emerging area of ‘large-scale data’ or the more vaguely defined ‘Big Data’ is a response to the increasing prevalence of computationally challenging datasets as arise in text analysis or web-scale prediction tasks, to give two examples. Here both n and p can run into the millions or more, particularly if interactions are considered. In these ‘large p , large n ’ regression scenarios, one can imagine situations where ordinary least squares (OLS) has competitive performance for prediction, but the sheer size of the data renders it infeasible for computational rather than statistical reasons.

An important feature of many large-scale datasets is that they are sparse: the overwhelming majority of entries in the design matrices are exactly zero. This is not to be confused with signal

sparsity, a common assumption in the high-dimensional context. Indeed, when the design matrix is sparse, having only a few variables that contribute to the response would make the expected response values of all observations with no non-zero entries for the important variables exactly the same; one expects that such a property would not be possessed by many datasets. However, similarly to the way in which many high-dimensional techniques exploit sparsity to improve statistical efficiency, one might hope that sparsity in the data could be leveraged to yield both computational and statistical improvements, and indeed we demonstrate in this work that this can be achieved.

When faced with such large-scale data, a sensible way to proceed is by first performing dimension reduction, that is by mapping the $n \times p$ design matrix \mathbf{X} to an $n \times d$ matrix \mathbf{S} with $d \ll p$. If the task to be performed with the original data was regression, one can then perform regression using the matrix \mathbf{S} rather than \mathbf{X} .

A remarkably effective way of doing this that is applicable when the design matrix is sparse and binary, is b -bit min-wise hashing [Li and König, 2011, Li et al., 2011]. The method is based on an earlier technique called min-wise hashing [Broder et al., 1998, Cohen et al., 2001, Datar and Muthukrishnan, 2002] and can also be viewed as part of a larger body of work on approximating kernel machines. Indeed the construction of \mathbf{S} has the following property: the dot product between any two rows of \mathbf{S} , $\mathbf{s}_i^T \mathbf{s}_j$, can approximate the *Jaccard similarity* or *resemblance* between the corresponding rows of \mathbf{X} , defined as $|\mathbf{z}_i \cap \mathbf{z}_j|/|\mathbf{z}_i \cup \mathbf{z}_j|$ where $\mathbf{z}_i = \{k : X_{ik} \neq 0\}$. In this way, one can approximate a kernel support vector machine (SVM) with a linear SVM on \mathbf{S} , for example.

Existing theory on b -bit min-wise hashing [Li and König, 2011] has focused on the variance and bias in the approximation of the kernel. However this alone does not fully explain the impressive empirical performance of b -bit min-wise hashing [Li et al., 2011, 2013]. Any prediction error bound for procedures applied to \mathbf{S} when the signal is generated by linear model, for example, would need to (implicitly at least) quantify the performance of the resemblance kernel in this setting; to the best of our knowledge, no such results for the resemblance kernel exist.

1.1 Our contributions

In this paper we derive finite-sample bounds on the expected risk of linear and logistic regression following dimension reduction through b -bit min-wise hashing under various different models. Our results show that the method, and hence also the resemblance kernel, are particularly suited to sparse data.

We describe the b -bit min-wise hashing algorithm in Section 2 and also discuss the connection to the resemblance kernel. In Section 3 we first study how well a linear combination of columns of \mathbf{S} can approximate a main effects signal in \mathbf{X} . We then explore how \mathbf{S} can also approximate main effects signals created using versions of \mathbf{X} whose rows have been scaled in certain ways. Such row normalisation is often performed on the original data as a pre-processing step, but the optimal normalisation to use is seldom known; our theory shows how b -bit min-wise hashing is able to in a sense automatically discover an appropriate scaling in several settings.

In Section 4.1 we study the performance of ordinary least squares, ridge regression and ℓ_2 -penalised logistic regression using the reduced design matrix it creates. Our results show in particular that if the original data are well-approximated by a linear model with coefficient vector β^* , then the expected mean-squared prediction error is bounded by a small constant times $\sqrt{q/n} \|\beta^*\|_2$, where q is the average number nonzero entries in the rows of \mathbf{X} . If the signal is spread out across many variables, $\|\beta^*\|_2$ will tend to be small and the scheme will perform well. We present similar results for logistic regression.

In Section 5 we show that interaction models in the original data can also be captured by main effects regression on the compressed data. Approximating these signals does not require a modification of the procedure, though one typically needs a larger dimensional mapping to reduce the error. Variable importance measures are discussed in Section 6. We conclude with a discussion in Section 7, and all proofs are collected in the appendix.

1.2 Related work

There is a huge variety of dimension reduction schemes across the statistics and computer science literature. Performing principal component analysis [Jolliffe, 1986] (PCA) and retaining only the first d components is one of the most popular methods. One drawback however in the large-scale data setting is that computing the principal components can be computationally demanding. The method of random projections, motivated by the celebrated Johnson–Lindenstrauss lemma [Johnson and Lindenstrauss, 1984], offers dimension reduction at a low computational cost. In this scheme, \mathbf{X} is mapped to \mathbf{XA} , where \mathbf{A} is a $p \times d$ matrix typically with i.i.d. random entries. Efficient implementations are discussed in Achlioptas [2001], Li et al. [2006b] and some numerical results on random projections and a wider literature review are in Fradkin and Madigan [2003], Vempala [2005]. The software package *Vowpal Wabbit* [Langford et al., 2007] is a popular learning system for large-scale datasets that uses sparse random projections.

A separate line of work has considered pre-multiplying \mathbf{X} with a random matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ to produce a reduced matrix $\mathbf{AX} \in \mathbb{R}^{m \times p}$, known as a *sketch*. Though the dimension p is not reduced, when n is large, performing OLS on the sketched matrix may be possible despite the computational infeasibility of applying least squares directly to \mathbf{X} . A number of works have studied properties sketched least squares (see Boutsidis and Drineas [2009], Drineas et al. [2011], Mahoney [2011], Pilanci and Wainwright [2015] and references therein) whilst Pilanci and Wainwright [2014] propose an iterative variant of this scheme. Yang et al. [2015] considers sketching ideas in the context of kernel ridge regression.

Approximating kernel methods using random feature expansions was studied by Rahimi and Recht [2007] who introduced the ‘random kitchen sink’ method for radial basis function kernels; Le et al. [2013] introduce a related scheme that further improves the computational efficiency. Similar methods for wider classes of kernels are developed in Shi et al. [2009], Weinberger et al. [2009], Vedaldi and Zisserman [2012], Kar and Karnick [2012], Li [2014].

Properties of b -bit min-wise hashing related to similarity search are studied in Li and König [2011]. Theory concerning its use for large-scale learning is presented in Li et al. [2011] which quantifies the mean and variance of entries in the Gram matrix \mathbf{SS}^T and its relationship to the resemblance kernel as well as providing comparisons with random projections and *Vowpal Wabbit*.

2 b -bit min-wise hashing

Given a sparse design matrix $\mathbf{X} \in \mathbb{R}^{n \times p}$, the aim of dimension reduction is to map this to a compressed matrix $\mathbf{S} \in \mathbb{R}^{n \times d}$, in a way that is computationally efficient and such that the relevant information in \mathbf{X} is preserved in \mathbf{S} . Section 2.2 describes the mapping to \mathbf{S} under b -bit min-wise hashing for binary data, as proposed in Li and König [2011] and Li et al. [2011]. The construction may seem unintuitive at first sight, but we will try to shed light on why the scheme works for linear and interaction models throughout the manuscript.

2.1 Notation

Given a matrix \mathbf{U} , we will write \mathbf{u}_i and \mathbf{U}_j for the i th row and j th column respectively, where both are to be regarded as column vectors. The ij th entry will be denoted U_{ij} . A vector of 1's will be denoted $\mathbf{1}$.

When the parentheses following probability and expectation signs, \mathbb{P} and \mathbb{E} , enclose multiple potential sources of randomness, we will sometimes add subscripts to indicate what is being considered as random. For example, if U and V are random variables, we may write $\mathbb{E}_U(U|V)$ for the conditional expectation of U given V , and $\mathbb{E}_{U,V}(U + V)$ for the expected value of $U + V$.

2.2 Construction of \mathbf{S} with b -bit min-wise hashing and binary variables

The compressed matrix \mathbf{S} generated by b -bit min-wise hashing consists of blocks of size 2^b , where we may choose the number of blocks L . Each block is created using a random permutation and the blocks of columns form a collection of L i.i.d. random matrices.

There are three steps to the construction.

Step 1: Generate a random permutation of the set $\{1, \dots, p\}$, π_l , and permute the columns of \mathbf{X} according to this permutation.

Step 2: Search along each row of the permuted design matrix (in order of increasing column index) and record in the vector $\mathbf{H}_l \in \mathbb{N}^n$ the indices of the variables (indexed as in the original order) with the first non-zero value or the vector $\mathbf{M}_l \in \mathbb{N}^n$ the indices of the variables (indexed as in the permuted order) with the first non-zero value.

Step 3: Form $\mathbf{S}_l \in \{0, 1\}^{n \times 2^b}$ with i th row given by the last b bits of the binary representation of the i th entry of \mathbf{M}_l . For example, when $b = 1$, all odd numbers in \mathbf{M}_l map to the vector $(0, 1)$, whereas all even numbers map to $(1, 0)$.

This construction is illustrated for a toy example in Table 1.

$\mathbf{X} = \begin{pmatrix} \cdot & 1 & \cdot & 1 \\ \cdot & \cdot & 1 & 1 \\ 1 & \cdot & 1 & \cdot \\ \cdot & 1 & 1 & \cdot \\ 1 & 1 & \cdot & \cdot \end{pmatrix} \xrightarrow{\pi_l=2314} \begin{pmatrix} \cdot & \cdot & \mathbf{1} & \mathbf{1} \\ \mathbf{1} & \cdot & \cdot & 1 \\ \mathbf{1} & 1 & \cdot & \cdot \\ \mathbf{1} & \cdot & 1 & \cdot \\ \cdot & \mathbf{1} & 1 & \cdot \end{pmatrix}$	$\mathbf{H}_l = \begin{pmatrix} 2 \\ 3 \\ 3 \\ 3 \\ 1 \end{pmatrix}, \mathbf{M}_l = \begin{pmatrix} 3 \\ 1 \\ 1 \\ 1 \\ 2 \end{pmatrix}$	$\mathbf{S}_l = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$
<p><i>Step 1:</i> non-zero indices whose variable indices will appear in \mathbf{H}_l in Step 2 are in bold.</p>	<p><i>Step 2.</i></p>	<p><i>Step 3.</i></p>

Table 1: Steps 1–3 applied to a toy example with $b = 2$. Dots represent zeroes.

We can think of each column of \mathbf{S}_l as representing different categories for the observations. The matrix \mathbf{S}_l itself codes for the assignment of the different rows of \mathbf{X} to the different categories. Different blocks \mathbf{S}_l then represent different random categorisations. Identical rows will always be assigned the same categories and the more different the rows are, the less likely they are to be assigned the same category. The notion of difference here is that of *resemblance*; see Section 2.4

Note that one would not necessarily follow the above steps when implementing b -bit min-wise hashing. In practice, one would not store the entire matrix of signs nor all the random permutations. In an implementation, hash functions [Carter and Wegman, 1979] would be used to create the matrix \mathbf{S} deterministically, though it is beyond the scope of this paper to go into the details; see Li et al. [2013] for more information and further computational improvements. With this approach, \mathbf{S} would be created row-by-row, and only a single observation from \mathbf{X} would need to be kept in memory at any one time. Furthermore, many rows could be created in parallel. Other ideas such as one-permutation hashing [Li et al., 2012] can also be used to speed up the pre-processing step.

2.3 Continuous data and additional randomisation

For continuous data, following Li et al. [2006a], we replace the map extracting the last b bits by L random maps in the following way. Fix b and let $\Psi \in \{1, \dots, 2^b\}^{p \times L}$ be a random matrix with independent entries each having the uniform distribution on the set $\{1, \dots, 2^b\}$. We then create \mathbf{S} by modifying the previous Step 3 to the following.

Step 3: Form $\mathbf{S}_l \in \{0, 1\}^{n \times 2^b}$ with i th row all zero except component $\Psi_{H_{il}}$ takes the value 1.

Step 4: If \mathbf{X} is not binary, multiply the i th row of \mathbf{S}_l by $X_{iH_{il}}$.

Let $\mathbf{z}_i = \{k : X_{ik} \neq 0\}$ be the set of variable indices whose entries have non-zero values for the i th observation. Performing the steps above for all $l = 1, \dots, L$, we get $n \times L$ matrices \mathbf{H} , and \mathbf{M} given by

$$H_{il} = \arg \min_{k \in \mathbf{z}_i} \pi_l(k), \quad (2.1)$$

$$M_{il} = \min_{k \in \mathbf{z}_i} \pi_l(k) = \pi_l(H_{il}), \quad (2.2)$$

The matrix \mathbf{S} is a binary $n \times 2^b L$ matrix. With a slight abuse of notation, we will denote by \mathbf{S}_{ilc} the c th entry in the l th block of \mathbf{S} :

$$S_{ilc} := S_{i(c+(l-1)2^b)} = X_{iH_{il}} \mathbb{1}_{\{\Psi_{H_{il}}=c\}}, \quad \text{for } c = 1, \dots, 2^b. \quad (2.3)$$

If not stated otherwise, we will work with this second randomised variation of b -bit min-wise hashing from now on. We emphasise that we do not make the claim this version is to be preferred over the original proposal of Li and König [2011] and Li et al. [2011]. We simply introduce the additional randomisation here to simplify the analysis. We note that the two versions are essentially identical for all practical purposes when b is not too large.

2.4 The resemblance kernel

We now briefly describe the connection between b -bit min-wise hashing and the resemblance kernel alluded to earlier. This is not needed for the rest of the paper, though it provides some intuition for the scheme. A more detailed analysis from this perspective is carried out by Li et al. [2011] and we refer the reader to Hofmann et al. [2008] for a review of kernel methods and the kernel trick.

Suppose \mathbf{X} is binary. Consider the normalised Gram matrix of the compressed design \mathbf{S} from (randomised) b -bit min-wise hashing, $\mathbf{S}\mathbf{S}^T/L$. The expected value of the ij th component may be calculated as follows.

$$\begin{aligned} \mathbb{E}_{\pi, \Psi}(\mathbf{s}_i^T \mathbf{s}_j / L) &= \frac{1}{L} \sum_{l=1}^L \sum_{c=1}^{2^b} \mathbb{E}_{\pi, \Psi}(\mathbb{1}_{\{\Psi_{H_{il}}=c\}} \mathbb{1}_{\{\Psi_{H_{jl}}=c\}}) \\ &= \mathbb{P}(\Psi_{H_{il}} = \Psi_{H_{jl}}) \\ &= \mathbb{P}(\Psi_{H_{il}} = \Psi_{H_{jl}} | H_{il} = H_{jl}) \mathbb{P}(H_{il} = H_{jl}) \\ &\quad + \mathbb{P}(\Psi_{H_{il}} = \Psi_{H_{jl}} | H_{il} \neq H_{jl}) \{1 - \mathbb{P}(H_{il} = H_{jl})\} \\ &= \frac{|\mathbf{z}_i \cap \mathbf{z}_j|}{|\mathbf{z}_i \cup \mathbf{z}_j|} (1 - 2^{-b}) + 2^{-b}. \end{aligned}$$

Thus the ij th entry is an average of L i.i.d. random variables with expectation a constant plus a constant times the resemblance between the i th and j th rows of \mathbf{X} . If an intercept term is included when regressing on \mathbf{S} , the additive constant plays no part, and the scaling would be absorbed into the scaling of the regression coefficients. We also note that when \mathbf{X} is continuous, the resulting kernel is similar to the the CoRE Type 2 kernel of Li [2014].

Now as the resemblance kernel is positive definite (see for example Li et al. [2011] for a short proof of this), the theory surrounding the kernel trick tells us that any ℓ_2 regularised regression on \mathbf{S} is effectively approximating a regularised regression on transformed data $\phi(\mathbf{x}_i)$ where $\phi : \{0, 1\}^p \rightarrow \mathcal{H}$ and \mathcal{H} is a high-dimensional inner product space (the feature space). This space may be taken to be a reproducing kernel Hilbert space (RKHS), and then ϕ and \mathcal{H} are uniquely defined.

Although this is encouraging, the kernel trick does not guarantee that regression on \mathbf{S} will necessarily have good predictive properties for models of interest. To gain a better understanding, we must study the regularisation properties of the resemblance kernel itself: what characterises those elements of the associated RKHS \mathcal{H} that have low norm and thus will be penalised less?

A direct analysis of the RKHS corresponding to the resemblance kernel in those terms seems challenging. We take a different approach and explicitly construct regression coefficients for \mathbf{S} that approximate signals of interest. By showing that particular signals can be approximated well, we are indirectly discovering elements of \mathcal{H} with low RKHS norm.

3 Approximation error

In this section, we present results that bound the expected prediction error when performing regression on the reduced design matrix \mathbf{S} in the contexts of the linear and logistic regression models. Note that throughout the rest of the manuscript, by b -bit min-wise hashing we are referring to the randomised variant described in Section 2.3. Let q_i be the number of non-zero entries in the i th row of \mathbf{X} , and let $\delta_i = q_i/p$ be the row sparsity. We will assume that the signal we wish to approximate for the i th observation takes the form

$$\kappa(\delta_i) \mathbf{x}_i^T \boldsymbol{\beta}^*. \tag{3.1}$$

Here $\boldsymbol{\beta}^* \in \mathbb{R}^p$ is an unknown vector of coefficients and the function κ allows the i th linear predictor to be scaled in a way which depends on the number of non-zero entries in the i th row of \mathbf{X} . Some normalisations of special interest include:

- (a) $\kappa(\delta)$ constant. This yields standard linear or logistic regression models.
- (b) $\kappa(\delta) \propto \delta^{-1/2}$. In text analysis with a bag of words representation of documents, rows of \mathbf{X} are often scaled to have the same ℓ_2 -norm to help balance situations when documents vary greatly in length [Banerjee et al., 2005]. When \mathbf{X} is binary, this is exactly achieved by taking $\kappa(\delta) = p^{-1/2}\delta^{-1/2}$, so $\kappa(\delta_i) = q_i^{-1/2}$.
- (c) $\kappa(\delta) \propto \delta^{-1}$. This leads to a ℓ_1 -norm scaling as opposed to the ℓ_2 -norm scaling mentioned above.

Throughout we will assume that $\mathbf{X} \in [-1, 1]^{n \times p}$, so the entries in \mathbf{X} are bounded. This covers the important case of binary design but also allows for real-valued entries.

The first step in obtaining our prediction error results is to construct a vector \mathbf{b}^* such that $\mathbf{s}_i^T \mathbf{b}^*$ is close to $\kappa(\delta_i) \mathbf{x}_i^T \boldsymbol{\beta}^*$ on average.

3.1 Un-scaled signals

We will first consider un-scaled signals where $\kappa(\delta)$ in (3.1) is a constant. Non-constant row-scaling is treated in more detail in the Section 3.2. To begin with we will assume that $q_i = q \geq 1$ for all $i = 1, \dots, n$, a restriction which simplifies the results but highlights some interesting properties of b -bit min-wise hashing. Unequal row sparsity is treated in detail in the appendix in Section 8.1.1 but a sketch of the results are given just below Theorem 1.

To simplify notation, we first introduce the following norm for $\boldsymbol{\beta} \in \mathbb{R}^p$,

$$\|\boldsymbol{\beta}\|_b^2 := \|\boldsymbol{\beta}\|_2^2 + (2^b - 2) \sum_{k=1}^p \frac{\|\mathbf{X}_k\|_2^2}{n} \beta_k^2. \quad (3.2)$$

When $b = 1$, $\|\boldsymbol{\beta}\|_b^2 = \|\boldsymbol{\beta}\|_2^2$. For larger values of b , the norm is influenced more heavily by the second term which can be seen to be the weighted version of the ℓ_2 -norm, where the weight of each variable is proportional to its squared ℓ_2 -norm. We will first discuss how well the original signal can be approximated with the column space of the map \mathbf{S} generated by the b -bit min-wise hashing operation.

Theorem 1. *Let \mathbf{S} be the matrix generated by b -bit min-wise hashing. Then there exists a vector $\mathbf{b}^* \in \mathbb{R}^{2^b L}$ with the following properties.*

(i) *The approximation is unbiased: $\mathbb{E}_{\pi, \Psi}(\mathbf{S}\mathbf{b}^*) = \mathbf{X}\boldsymbol{\beta}^*$.*

(ii) *The norm is bounded by*

$$\mathbb{E}_{\pi, \Psi}(\|\mathbf{b}^*\|_2^2) \leq \frac{(2 - \delta)q}{L(1 - 2^{-b})} \|\boldsymbol{\beta}^*\|_2^2.$$

(iii) *The approximation error is bounded by*

$$\frac{1}{n} \mathbb{E}_{\pi, \Psi}(\|\mathbf{S}\mathbf{b}^* - \mathbf{X}\boldsymbol{\beta}^*\|_2^2) \leq \frac{(2 - \delta)q}{2^b L(1 - 2^{-b})} \|\boldsymbol{\beta}^*\|_b^2.$$

Specifically, for $b = 1$, $\mathbb{E}_{\pi, \Psi}(\|\mathbf{S}\mathbf{b}^ - \mathbf{X}\boldsymbol{\beta}^*\|_2^2)/n \leq (2 - \delta)q\|\boldsymbol{\beta}^*\|_2^2/L$.*

A form of the approximation error (iii) and the norm bound (ii) continue to be valid in the non-equal sparsity case under a mild restriction on the size of L , where we get instead of (iii) the bound

$$\frac{1}{n} \mathbb{E}_{\pi, \Psi} (\|\mathbf{S}\mathbf{b}^* - \mathbf{X}\boldsymbol{\beta}^*\|_2^2) \leq \frac{6\bar{q}}{2^b L (1 - 2^{-b})} \|\boldsymbol{\beta}^*\|_2^2,$$

where \bar{q} is the the average of the q_i ; see Theorem 12 for details.

The results above show that the signal $\mathbf{X}\boldsymbol{\beta}^*$ can be well approximated by a linear combination of the columns in the matrix \mathbf{S} if we generate a sufficiently large number of permutations L , especially for sparse data matrices. Another useful property of \mathbf{b}^* here, aside from the approximation accuracy it delivers, is given in (ii): on average, $\|\mathbf{b}^*\|_2^2$ is small when L is large. This proves to be useful when studying the application of ridge regression.

Whilst the bound on the expectation of $\|\mathbf{b}^*\|_2^2$ is almost constant as b changes, the approximation error bound (iii) does vary with b . Consider the case where \mathbf{X} is binary and let $\gamma_k = \|\mathbf{X}_k\|_2^2/n$ be the column sparsity. Typically one would expect $\|\boldsymbol{\beta}^*\|_2^2$ to be significantly larger than $\sum_{k=1}^p \gamma_k \beta_k^{*2}$ and thus increasing b by 1 almost halves the approximation error when b is small.

A proof of Theorem 1 is given in Section 8.1; here we briefly sketch some of the main ideas. Note that

$$\mathbb{E}_{\pi, \Psi} (\mathbf{S}\mathbf{b}^*) = \sum_{l=1}^L \mathbb{E}_{\pi, \Psi} \left(\sum_{c=1}^{2^b} \mathbf{S}_{lc} b_{lc}^* \right). \quad (3.3)$$

We construct \mathbf{b}^* with the following two properties: each of the L blocks of \mathbf{b}^* are i.i.d. with the l th block only depending on π_l and Ψ_l ; and each of the L summands in (3.3) equals $\mathbf{X}\boldsymbol{\beta}^*/L$. With each of the L summands being unbiased in this way, we see that the approximation error is controlled by the variance of the sum; this variance scales as $1/L$ since the summands are i.i.d.

At first sight it may seem surprising that it is possible to exhibit a \mathbf{b}^* with each block having the unbiasedness property discussed above. However the following construction gives an indication of the possibilities. Using our convention that the c th component of the l th block of \mathbf{b}^* is indexed as $b_{lc}^* := b_{c+(l-1)2^b}^*$, consider taking

$$b_{lc}^* = \frac{q}{L} \sum_{k=1}^p \beta_k^* \frac{\mathbb{1}_{\{\Psi_{lk}=c\}} - 2^{-b}}{1 - 2^{-b}}. \quad (3.4)$$

Then writing $\boldsymbol{\psi} = \Psi_1$, $\pi = \pi_1$, $H_i = H_{i1}$ we have

$$\begin{aligned} \frac{L}{q} \mathbb{E}_{\pi, \boldsymbol{\psi}} \left(\sum_{c=1}^{2^b} S_{lc} b_{lc}^* \right) &= \mathbb{E}_{\pi, \boldsymbol{\psi}} \left(\sum_{c=1}^{2^b} \sum_{j=1}^p X_{ij} \mathbb{1}_{\{H_i=j, \psi_j=c\}} \sum_{k=1}^p \beta_k^* \frac{\mathbb{1}_{\{\psi_k=c\}} - 2^{-b}}{1 - 2^{-b}} \right) \\ &= \mathbb{E}_{\pi, \boldsymbol{\psi}} \left(\sum_{j=1}^p X_{ij} \mathbb{1}_{\{H_i=j\}} \sum_{k=1}^p \beta_k^* \frac{\mathbb{1}_{\{\psi_k=\psi_j\}} - 2^{-b}}{1 - 2^{-b}} \right). \end{aligned} \quad (3.5)$$

Now since $\mathbb{E}_{\boldsymbol{\psi}} \{(\mathbb{1}_{\{\psi_k=\psi_j\}} - 2^{-b})/(1 - 2^{-b})\} = \mathbb{1}_{\{k=j\}}$ we see the above display equals

$$q \sum_{k=1}^p X_{ik} \beta_k^* \mathbb{P}_{\pi}(H_i = k) = \mathbf{X}\boldsymbol{\beta}^*.$$

The final line uses the fact that for k with $X_{ik} \neq 0$, $\mathbb{P}_\pi(H_i = k)$ is the reciprocal of the number of non-zero entries in the i th row of \mathbf{X} ; with our simplifying assumption of equal row sparsity, this is precisely $1/q$. Note one could scale the rows of \mathbf{S} according to the number of non-zeroes in each row to achieve unbiasedness in the case of unequal row sparsity. However as shown in Section 8.1.1, it turns out that by incurring some bias one can still keep the approximation error low even in this situation without having to perform any sort of scaling.

The form of \mathbf{b}^* used in the proof of Theorem 1 differs slightly from that in (3.4) by introducing a random weight multiplying each coefficient that decays as $\pi_l(k)$ increases. This reduces the variance and yields the approximation error in (iii) that has a factor q rather than the factor of p which would be obtained from (3.4).

3.2 Row-scaled signals

We now turn to the more general setting with unequal row sparsity and signal given by (3.1). We consider the family of scaling functions $\delta \mapsto (\delta_{\min}/\delta)^a$ where $\delta_{\min} = \min_i \delta_i$, for $1/2 \leq a \leq 1$. Including δ_{\min} in the scaling functions means that were the row sparsity to be equal, the approximation error here would be of the same form as that considered in Theorems 1. We could alternatively replace δ_{\min} with the average of the δ_i for the same effect, but using δ_{\min} helps to simplify the results. Writing $q_{\min} = \min_i q_i$, we have the following results.

Theorem 2. *Let $L \geq 5$ and assume $\delta_{\min} \leq 1/2$ if $a = 1/2$, and $L > 2/(2a - 1)$ if $a > 1/2$. Then there exists $\mathbf{b}^* \in \mathbb{R}^L$ depending on a such that the approximation error satisfies*

$$\frac{1}{n} \sum_{i=1}^n \mathbb{E}_{\pi, \Psi} [\{(\delta_{\min}/\delta_i)^a \mathbf{x}_i^T \boldsymbol{\beta}^* - \mathbf{s}_i^T \mathbf{b}^*\}^2] \leq \begin{cases} \frac{q_{\min}}{2^b L(1 - 2^{-b})} \|\boldsymbol{\beta}^*\|_b^2 \log\{4 \log(L)/\delta_{\min}\} & \text{if } a = 1/2, \\ \frac{q_{\min}}{2^b L(1 - 2^{-b})} \|\boldsymbol{\beta}^*\|_b^2 \frac{1}{2a - 1} [\log\{2(2a - 1)L\}]^{2a-1} & \text{if } 1/2 < a \leq 1, \end{cases}$$

and the norm of \mathbf{b}^* is bounded in expectation by

$$\mathbb{E}_{\pi, \Psi} (\|\mathbf{b}^*\|_2^2) \leq \begin{cases} \frac{q_{\min} \log\{4 \log(L)/\delta_{\min}\}}{L(1 - 2^{-b})} \|\boldsymbol{\beta}^*\|_2^2 & \text{if } a = 1/2, \\ \frac{1}{2a - 1} \frac{q_{\min} [\log\{2(2a - 1)L\}]^{2a-1}}{L(1 - 2^{-b})} \|\boldsymbol{\beta}^*\|_2^2 & \text{if } 1/2 < a \leq 1. \end{cases}$$

The min-wise hashing based dimension reduction scheme appears to be well-suited to approximating signals scaled by a power of the sparsity, with the approximation error only incurring a further multiplicative term involving $\log(L)$ compared to the results of Theorem 1.

We now briefly outline how we construct coefficient vectors \mathbf{b}^* achieving the bounds above. Consider the following refinement of (3.4):

$$b_{ic}^* = \frac{1}{L} \sum_{k=1}^p \beta_k^* \frac{\mathbb{1}_{\{\Psi_{lk}=c\}} - 2^{-b}}{1 - 2^{-b}} w_{\pi_l(k)},$$

where $\mathbf{w} \in \mathbb{R}^p$ is a vector of non-negative weights. Arguing as in (3.5) but replacing $q\beta_k^*$ with $\beta_k^* w_{\pi(k)}$ we arrive at

$$L\mathbb{E}_{\pi, \psi} \left(\sum_{c=1}^{2^b} S_{1c} b_{1c}^* \right) = \sum_{k=1}^p X_{ik} \beta_k^* \mathbb{E}_{\pi} (\mathbb{1}_{\{H_i=k\}} w_{\pi(k)}).$$

Recall that writing $M_i = M_{i1}$, $M_i = \pi(H_i)$, the position of the first non-zero entry in row i under permutation π . Note that H_i and M_i are independent. Now for large p , M_i behaves roughly like a geometric random variable with parameter δ_i . Thus for k with $X_{ik} \neq 0$,

$$\mathbb{E}_{\pi} (\mathbb{1}_{\{H_i=k\}} w_{\pi(k)}) = \mathbb{E}_{\pi} (\mathbb{1}_{\{H_i=k\}} w_{M_i}) \approx \frac{1}{p\delta_i} \sum_{\ell=1}^p w_{\ell} \delta_i (1 - \delta_i)^{\ell-1} = \frac{1}{p} \sum_{\ell=1}^p w_{\ell} (1 - \delta_i)^{\ell-1}.$$

If $w_{\ell+1} = p(-1)^{\ell} \kappa^{(\ell)}(1)/\ell!$ we see that the RHS resembles a Taylor series of $\kappa(\delta_i)$ about 1. In this way we can approximate a large family of row-scaled signals.

4 Prediction error

The approximation error results in the three previous sections allow us to derive bounds on the prediction errors for linear and logistic regression models with potentially row-scaled data. Here we will present results under the assumption of q non-zero entries per row and also where the scaling function κ is proportional to the square-root function

$$\kappa_0(\delta) = \sqrt{\delta_{\min}/\delta}. \quad (4.1)$$

However, all of the approximation error results can be extended to results on prediction error via general theorems on prediction error we present in Section 8.2. In particular, Theorem 12 can be used to show that versions of the equal row sparsity results hold more generally with q replaced by the average number of non-zeroes per row \bar{q} provided L is not excessively large.

4.1 Linear regression models

Assume we have the following approximately linear model:

$$Y_i = \alpha^* + \kappa(\delta_i) \mathbf{x}_i^T \boldsymbol{\beta}^* + \varepsilon_i, \quad i = 1, \dots, n. \quad (4.2)$$

Here α^* is the intercept and $\mathbf{x}_i \in [-1, 1]^p$. We assume that the random noise $\boldsymbol{\varepsilon} \in \mathbb{R}^n$ satisfies $\mathbb{E}(\varepsilon_i) = 0$, $\mathbb{E}(\varepsilon_i^2) = \sigma^2$ and $\text{Cov}(\varepsilon_i, \varepsilon_j) = 0$.

Our results here give bounds on a mean-squared prediction error (MSPE) of the form

$$\text{MSPE}((\hat{\alpha}, \hat{\mathbf{b}})) := \frac{1}{n} \sum_{i=1}^n \mathbb{E}_{\boldsymbol{\varepsilon}, \boldsymbol{\pi}, \boldsymbol{\Psi}} \{ (\alpha^* + \kappa(\delta_i) \mathbf{x}_i^T \boldsymbol{\beta}^* - \hat{\alpha} - \mathbf{S} \hat{\mathbf{b}})^2 \} \quad (4.3)$$

where $\hat{\alpha}$ and $\hat{\mathbf{b}}$ are the estimated intercept and regression coefficients arising from regression on \mathbf{S} . Note we consider a denoising-type error: the error on the data used to fit the regression coefficients. Bounds on the prediction error at new observations would require conditions on the distribution of observations and we have avoided making any such assumptions for the results here.

4.1.1 Ordinary least squares

Perhaps the simplest way to estimate the linear model is to apply a least squares estimator,

$$(\hat{\alpha}, \hat{\mathbf{b}}) := \arg \min_{(\alpha, \mathbf{b}) \in \mathbb{R} \times \mathbb{R}^{2^b L}} \|\mathbf{Y} - \alpha \mathbf{1} - \mathbf{S}\mathbf{b}\|_2^2, \quad (4.4)$$

to the matrix \mathbf{S} . We have the following theorem.

Theorem 3. *Let $(\hat{\alpha}, \hat{\mathbf{b}})$ be the least squares estimator (4.4). We have the bound*

$$\text{MSPE}((\hat{\alpha}, \hat{\mathbf{b}})) \leq \frac{C}{2^b L (1 - 2^{-b})} \|\boldsymbol{\beta}^*\|_b^2 + 2^b L \frac{\sigma^2}{n}.$$

For equal row sparsity δ we have $C = (2 - \delta)q$. For unequal row sparsity, when $\kappa = \kappa_0$ as in (4.1), the result holds for $C = q_{\min} \log\{4 \log(L)/\delta_{\min}\}$.

An optimal choice L_b^* of L will balance the approximation error and variance contributions (first and second term on the right hand side respectively). In the equal row sparsity we arrive at

$$L_b^* = \frac{\sqrt{(2 - \delta)qn}}{2^b \sqrt{1 - 2^{-b}}} \|\boldsymbol{\beta}^*\|_b$$

which yields an optimal MSPE of the order $\sigma \sqrt{q/n} \|\boldsymbol{\beta}^*\|_b$. If we ignore log terms the rate is analogous in the case of uneven row-sparsity. The slow rate in n seems unavoidable if we do not make stronger conditions on the design. Indeed, a similar error rate is obtained in Theorem 21 of Maillard and Munos [2012] and in Kaban [2014] for OLS following dimension reduction by random projections. More precisely: projecting K times with a random projection, followed by an OLS estimation is shown in Kaban [2014] to lead to a bound on MSPE of

$$\frac{1}{K} \|\boldsymbol{\beta}^*\|_{\kappa}^2 + K \frac{\sigma^2}{n}, \quad (4.5)$$

where the norm $\|\cdot\|_{\kappa}$ depends on the eigenvalue structure of the design matrix. In contrast the bound we have above for min-wise hashing depends on the sparsity q through the constant C . The bound (4.5) is otherwise structurally identical to the bound for b -bit min-wise hashing above, and the role of the number L of projections is now taken by the number K of random projections. The optimal values of K and L are both of order \sqrt{n} , leading to the same convergence rate of the risk as $n \rightarrow \infty$.

To better understand the implications of Theorem 3, it is helpful to fix the size of the signal so that $\|\mathbf{X}\boldsymbol{\beta}^*\|_2^2/n = 1$, and look at whether we can show consistency of the method as both $p, n \rightarrow \infty$. If the signal is spread out and all variables have the same sparsity, $\|\boldsymbol{\beta}^*\|_b$ will be of order $\sqrt{p/q}$ and the MSPE will vanish when $p/n \rightarrow 0$, which excludes the high-dimensional setting.

However, now assume that the signal is concentrated on a fixed set of variables. The norm $\|\boldsymbol{\beta}^*\|_b$ is then constant as p increases and all that is required for consistency is $q/n \rightarrow 0$ (or $q_{\min}/n \rightarrow 0$ for the more general case of uneven row-sparsity).

An interesting scenario is one of increasing variable sparseness. In many applications, the more predictor variables are added the sparser they tend to become. In text analysis, the first block of predictor variables might encode the presence of individual words. The next block might code for

bigrams and the following, higher order N -grams. With this design, predictor variables in each successive block become sparser than the previous. It is then interesting to consider how much the MSPE can increase if we add a block with many sparse variables which contain no additional signal contribution. The result above indicates that the MSPE only increases as \sqrt{q} . Adding a block of several million (sparse) bigrams might thus have the same statistical effect as adding several thousand (denser) unigrams (individual words).

We now comment the optimal choice of L and computational complexity. If we assume fixed $\|\boldsymbol{\beta}^*\|_2$ and $n = O(q)$, which is all that would be required to keep the prediction error bounded asymptotically, then the optimal dimension of the min-wise projection scales as $L_b^* = O(q)$, considering b fixed here. This dimension will in general be a substantial reduction over the original dimension of the data, p , and would result in a corresponding large reduction in the computational cost of regression. Indeed, ridge regression or the LAR algorithm [Efron et al., 2004] applied to \mathbf{X} would have complexity $O(q^2p)$, and one would expect that the Lasso [Tibshirani, 1996] would have similar computational cost. In contrast OLS applied to \mathbf{S} would only require $O(q^3)$ operations, an improvement of q/p . The discussion above considered an optimal choice of $L \approx L_b^*$. Even if we cannot afford to work with the optimal dimension L_b^* for computational reasons, the bound will still be useful for smaller values of L . The guarantee on prediction accuracy could not be obtained if, for example, simply a random subset of L predictors were chosen and the remaining ones discarded.

The dependence of the bound on b is also interesting: a minimum value occurs for $b = 1$. However, this would imply a larger value of L_b^* . Note the memory requirement for storing \mathbf{S} would be $O(nL_b^*b)$ as b bits would be required to store the locations of each of the nL_b^* nonzeros. We see that with a constraint on nbL or on the number of permutations L , larger values of b are more favourable, particularly with high sparsity, as this would tend to make $\|\boldsymbol{\beta}^*\|_b$ not much larger than $\|\boldsymbol{\beta}^*\|_2$. A different perspective on the optimal choice of b based on the variance of inner products of rows of \mathbf{S} is taken in Li and König [2011], with similar conclusions.

4.1.2 Ridge regression

Instead of using a least-squares estimator on the transformed data matrix \mathbf{S} we can also apply ridge regression [Hoerl and Kennard, 1970]. For a given $\lambda > 0$, the regression coefficients are found by

$$(\hat{\alpha}_\lambda, \hat{\mathbf{b}}_\lambda) := \arg \min_{(\alpha, \mathbf{b}) \in \mathbb{R} \times \mathbb{R}^L} \|\mathbf{Y} - \hat{\alpha}\mathbf{1} - \mathbf{S}\mathbf{b}\|_2^2 \text{ such that } \|\mathbf{b}\|_2^2 \leq \lambda, \quad (4.6)$$

The theorem below gives a bound on the MSPE of $(\hat{\alpha}, \hat{\mathbf{b}}_\lambda)$.

Theorem 4. *There exist regularisation parameters λ depending on $\boldsymbol{\beta}^*$ and \mathbf{S} such that*

$$\text{MSPE}((\hat{\alpha}_\lambda, \hat{\mathbf{b}}_\lambda)) \leq \sigma \sqrt{\frac{2C}{(1-2^{-b})n}} \|\boldsymbol{\beta}^*\|_2 + \frac{C}{2^b L (1-2^{-b})} \|\boldsymbol{\beta}^*\|_b^2 + \frac{\sigma^2}{n}.$$

Here the value of C is defined as in Theorem 3 by $C = (2 - \delta)q$ for equal row sparsity δ and $C = q_{\min} \log\{4 \log(L)/\delta_{\min}\}$ for $\kappa = \kappa_0$ and unequal row-sparsity.

The ridge regression result for large L is similar to that for OLS with an optimal L_b^* , though there is a small difference: the leading terms are $\sigma \|\boldsymbol{\beta}^*\|_2 \sqrt{q/n}$ and $\sigma \|\boldsymbol{\beta}^*\|_b \sqrt{q/n}$ respectively. Ridge regression takes advantage of the fact that not only do we have a \mathbf{b}^* such that $\mathbf{S}\mathbf{b}^*$ and $\mathbf{X}\boldsymbol{\beta}^*$ are close, we also know that there is a \mathbf{b}^* with this property that has low ℓ_2 -norm. Our bound on the

expected squared ℓ_2 -norm of \mathbf{b}^* ((ii) in Theorem 1) does not depend much on b . In contrast OLS only makes use of the approximation error result, (iii) in Theorem 1.

Note that when L is large, regardless of the value of b , ridge regression on \mathbf{S} approximates a kernel ridge regression using the resemblance kernel (see Section 2.4). The MSPE of a kernel ridge regression with the resemblance kernel should of course not depend on b , and this observation largely agrees with our result.

Another key difference between ridge regression and OLS here is the following: achieving a good prediction error with OLS hinges on a careful choice of L . In contrast, with ridge regression, L can (and should) be chosen very large, from a purely statistical point of view. However, the constraint on the ℓ_2 -norm of $\hat{\mathbf{b}}$ needs to be chosen carefully with ridge regression, typically by cross-validation. In practice, the number L of dimensions can be chosen as large as possible according to the available computational budget.

4.2 Logistic regression

We give an analogous result to Theorem 4 for classification problems under logistic loss. Let $\mathbf{x}_i \in [-1, 1]^p$ and let $\mathbf{Y} \in \{0, 1\}^n$ be an associated vector of class labels. We assume the model

$$Y_i \sim \text{Bernoulli}(p_i); \quad \log\left(\frac{p_i}{1-p_i}\right) = \kappa(\delta_i) \mathbf{x}_i^T \boldsymbol{\beta}^*, \quad (4.7)$$

with the Y_i independent for $i = 1, \dots, n$. Note that we have omitted the separate intercept term for simplicity.

Here we consider a linear classifier constructed by ℓ_2 -constrained logistic regression. One can obtain a similar result for unconstrained logistic regression based on Lemma 6.6 of Bühlmann and van de Geer [2011], but we do not pursue this further here. Define

$$\hat{\mathbf{b}}_\lambda = \arg \min_{\mathbf{b}} \frac{1}{n} \sum_{i=1}^n [-Y_i \mathbf{s}_i^T \mathbf{b} + \log\{1 + \exp(\mathbf{s}_i^T \mathbf{b})\}] \quad \text{such that} \quad \|\mathbf{b}\|_2^2 \leq \lambda. \quad (4.8)$$

Let $\mathcal{E}(\hat{\mathbf{b}}_\lambda)$ denote the excess risk of $\hat{\mathbf{b}}_\lambda$ under logistic loss, so

$$\mathcal{E}(\hat{\mathbf{b}}_\lambda) = \frac{1}{n} \sum_{i=1}^n [-p_i \mathbf{s}_i^T \hat{\mathbf{b}}_\lambda + \log\{1 + \exp(\mathbf{s}_i^T \hat{\mathbf{b}}_\lambda)\}] - \frac{1}{n} \sum_{i=1}^n [-p_i \kappa(\delta_i) \mathbf{x}_i^T \boldsymbol{\beta}^* + \log\{1 + \exp(\kappa(\delta_i) \mathbf{x}_i^T \boldsymbol{\beta}^*)\}]. \quad (4.9)$$

We can now state the analogous result to Theorem 4.

Theorem 5. Define $\tilde{p} \in \mathbb{R}$ by

$$\tilde{p} := \frac{1}{n} \sum_{i=1}^n p_i(1-p_i) \leq \frac{1}{2}. \quad (4.10)$$

Then we have that there exists a λ depending $\boldsymbol{\beta}^*$ and \mathbf{S} such that

$$\mathbb{E}_{\mathbf{Y}, \boldsymbol{\pi}, \boldsymbol{\Psi}} \{\mathcal{E}(\hat{\mathbf{b}}_\lambda)\} \leq \sqrt{\frac{2\tilde{p}C}{(1-2^{-b})n}} \|\boldsymbol{\beta}^*\|_2 + \frac{C}{2^{b+2}L(1-2^{-b})} \|\boldsymbol{\beta}^*\|_b^2.$$

Here the value of C is defined as in Theorem 3 by $C = (2-\delta)q$ for equal row sparsity δ and $C = q_{\min} \log\{4 \log(L)/\delta_{\min}\}$ for $\kappa = \kappa_0$ and unequal row-sparsity.

The result illustrates that the usefulness of b -bit min-wise hashing is not limited to regression problems. In fact, most applications are classification problems [Li and König, 2011] and our analysis of b -bit min-wise hashing here gives a theoretical explanation for its performance in these cases.

5 Interaction models

One of the compelling aspects of regression and classification with b -bit min-wise hashing is the fact that a particular form of interactions between variables can be fitted. This does not require any change in the procedure other than a possible increase in L . To be clear, in order to capture interactions with b -bit min-wise hashing, just as in the main effects case, we create a reduced matrix \mathbf{S} and then fit a main effects model to \mathbf{S} . The dimension of the compressed data, $2^b L$, can still be substantially smaller than the $O(p^2)$ number of coefficients that would need to be estimated if the interactions were modelled in the conventional way, and so the resulting computational advantage can be very large.

Note that in situations where the number of original predictors, p , may be manageable, including interactions explicitly can quickly become computationally infeasible. For example, if we start with, 10^5 variables, the two-way interactions number more than a billion. For larger values of p , even methods such as Random Forest [Breiman, 2001] or Rule Ensembles [Friedman and Popescu, 2008] would suffer similar computational problems.

We now describe a type of interaction model that can be fitted with b -bit min-wise hashing. Let $\mathbf{f}^* \in \mathbb{R}^n$ be given by

$$f_i^* = \sum_{k=1}^p X_{ik} \theta_k^{*,(1)} + \sum_{k,k_1=1}^p X_{ik} \mathbb{1}_{\{X_{ik_1}=0\}} \Theta_{k,k_1}^{*,(2)}, \quad i = 1, \dots, n, \quad (5.1)$$

where $\boldsymbol{\theta}^{*,(1)} \in \mathbb{R}^p$ is a vector of coefficients for the main effects terms, and $\boldsymbol{\Theta}^{*,(2)} \in \mathbb{R}^{p \times p}$ is a matrix of coefficients for interactions whose diagonal entries are zero. As elsewhere in the paper, throughout this section we will assume that $\mathbf{X} \in [-1, 1]^{n \times p}$. Note that if \mathbf{X} were a binary matrix, then (5.1) parametrises (in fact over-parametrises) all linear combinations of bivariate functions of predictors; that is all possible two-way interactions are included in the model.

In general, the interaction model includes the tensor product of the set of original variables with the columns of an $n \times p$ matrix with ik th entry $\mathbb{1}_{\{X_{ik}=0\}}$. The value zero is thus given a special status and the model seems particularly appropriate in the sparse design setting we are considering here.

5.1 Approximation error

We will assume that the number of non-zero entries in each row of \mathbf{X} is $q \geq 1$. However, we believe our proof techniques can be extended to the unequal sparsity and unknown row scaling scenario dealt with in Section 3.2. Furthermore, for technical reasons, we assume here that $p \geq 3$.

Let Θ^* collect together $\theta^{*,(1)}$ and $\Theta^{*,(2)}$ and define the following norms analogously to (3.2):

$$\|\Theta^*\| := \|\theta^{*,(1)}\|_2 + \left(2(2-\delta)q \sum_{k,k_1,k_2} \left| \Theta_{kk_1}^{*,(2)} \Theta_{kk_2}^{*,(2)} \right| \right)^{1/2}, \quad (5.2)$$

$$\|\Theta^*\|_b := \|\theta^{*,(1)}\|_b + \left\{ 2(2-\delta)q \left(\sum_{k,k_1,k_2} \left| \Theta_{kk_1}^{*,(2)} \Theta_{kk_2}^{*,(2)} \right| + \delta(2^b-2) \sum_{k,k_1,k_2} \frac{\|\mathbf{X}_k\|_2^2}{n} \left| \Theta_{kk_1}^{*,(2)} \Theta_{kk_2}^{*,(2)} \right| \right) \right\}^{1/2}. \quad (5.3)$$

Theorem 6. *Suppose we have exactly q non-zero entries in each row of \mathbf{X} . Then there exists a vector $\mathbf{b}^* \in \mathbb{R}^{2^b L}$ with the following properties:*

(i) *The approximation is unbiased, $\mathbb{E}_{\pi, \Psi}(\mathbf{S}\mathbf{b}^*) = \mathbf{f}^*$.*

(ii) *The ℓ_2 -norm is bounded by*

$$\mathbb{E}_{\pi, \Psi}(\|\mathbf{b}^*\|_2^2) \leq \frac{(2-\delta)q}{L(1-2^{-b})} \|\Theta^*\|^2.$$

(iii) *The approximation error is bounded by*

$$\mathbb{E}_{\pi, \Psi}(\|\mathbf{S}\mathbf{b}^* - \mathbf{f}^*\|_2^2)/n \leq \frac{(2-\delta)q}{2^b L(1-2^{-b})} \|\Theta^*\|_b^2.$$

The bound on the approximation error in (iii) is most suited to situations where there are a fixed number of interaction terms, so

$$\sum_{k,k_1,k_2} \left| \Theta_{kk_1}^{*,(2)} \Theta_{kk_2}^{*,(2)} \right| = O(1). \quad (5.4)$$

Then we see that the contribution of the interaction terms to the bound on the approximation error is of order q^2 . On the other hand, if we are considering a growing number of many small interaction terms, much tighter bounds than that given by (iii) can be obtained. The results for interaction models corresponding to Theorems 3, 4 and 5 now follow.

5.2 Prediction error

We now present results for linear and logistic regression models where the signal involves interactions.

5.2.1 Linear regression models

Assume the model (4.2) and define the MSPE by (4.3) but in both cases with $\mathbf{X}\boldsymbol{\beta}^*$ now replaced by \mathbf{f}^* (5.1). As in the previous section, we will assume that \mathbf{X} has q non-zero entries in each row. When OLS estimation is used, we have the following result.

Theorem 7. *Let $(\hat{\alpha}, \hat{\mathbf{b}})$ be the least squares estimator (4.4). Then*

$$\text{MSPE}((\hat{\alpha}, \hat{\mathbf{b}})) \leq \frac{(2-\delta)q}{2^b L(1-2^{-b})} \|\Theta^*\|_b^2 + 2^b L \frac{\sigma^2}{n}.$$

To interpret the result, consider a situation where there are a fixed number of interaction and main effects of fixed size, so in particular (5.4) holds. Then treating b as fixed, the optimal L , $L^* = O(\sqrt{q^2 n / \sigma})$. If n, q and p increase by collecting new data and adding uninformative variables, then in order for the MSPE to vanish asymptotically, we require $q^2/n \rightarrow 0$. Compare this to the corresponding requirement of OLS applied to \mathbf{X} , that $p^2/n \rightarrow 0$. Particularly in situations of increasing variable sparseness, as discussed in Section 4.1.1, this can amount to a large statistical advantage.

The computational gains can be equally great. If, for example, $n \approx q^2$, then $L^* = O(q^2)$. If ridge regression were applied to \mathbf{X} augmented by $O(p^2)$ interaction terms, the number of operations required would be $O(p^2 q^4)$; OLS using \mathbf{S} has complexity $O(q^6)$. If instead $n \approx p^2$, then regression with explicitly coded interaction terms would have complexity $O(p^6)$, whilst with the compressed data this would be reduced to $O(p^4 q^2)$.

As in the main effects case, the ridge regression result is similar.

Theorem 8. *Let the ridge regression estimator be given by (4.6). There exists λ depending on \mathbf{f}^* and \mathbf{S} such that we have*

$$\text{MSPE}((\hat{\alpha}, \hat{\mathbf{b}})) \leq \sigma \sqrt{\frac{(2-\delta)q}{n(1-2^{-b})}} \|\Theta^*\| + \frac{(2-\delta)q}{2^b L(1-2^{-b})} \|\Theta^*\|_b^2 + \frac{\sigma^2}{n}.$$

Similarly to Theorem 4 the result here suggests choosing a large L is always better from a statistical point of view. However, for computational reasons, it may not be possible to take L much larger than L^* .

5.2.2 Logistic regression

Here we assume the model (4.7) and define the excess risk by (4.9), but in both cases with $\mathbf{X}\beta^*$ replaced by \mathbf{f}^* .

Theorem 9. *Define $\tilde{p} \in \mathbb{R}$ as in (4.10) and the ℓ_2 -penalised logistic regression estimator as in (4.8). Then we have that there exists λ such that*

$$\mathbb{E}_{\mathbf{Y}, \pi, \Psi} \{\mathcal{E}(\hat{\mathbf{b}}_\lambda)\} \leq \sigma \sqrt{\frac{\tilde{p}(2-\delta)q}{n(1-2^{-b})}} \|\Theta^*\| + \frac{(2-\delta)q}{2^{b+2} L(1-2^{-b})} \|\Theta^*\|_b^2.$$

One could continue to look at higher-order interaction models by adding three-way interactions in (5.1) and adapting (5.2) and (5.3) in suitable ways. However, being able to show that two-way interaction models can be fitted with b -bit min-wise hashing may well be sufficient for most applications.

6 Extensions

6.1 Variable importance

Typically prediction, rather than model selection, is the primary goal in large-scale applications with sparse data, one reason for this being that we cannot expect a very small subset of variables to approximate the signal well when the design matrix is sparse. Nevertheless, it is often illuminating

to study the influence of specific variables or look for the variables that have the largest influence on predictions. Indeed, such study is often undertaken following applications of Random Forest [Breiman, 2001], where several variable importance measures allow practitioners to better interpret the fits produced.

We now describe how importance measures can be obtained for b -bit min-wise hashing as described in Section 2.3. Let $\hat{f} : \mathbb{R}^p \rightarrow \mathbb{R}$ be the regression function created following regression on b -bit min-wise hashed data, and let $\hat{f}_i := \hat{f}(\mathbf{x}_i)$. Furthermore, for $k = 1, \dots, p$, let $\hat{f}^{(-k)} := \hat{f}(\mathbf{x}_i^{(-k)})$, where $\mathbf{x}_i^{(-k)}$ is equal to \mathbf{x}_i but with k th component set to zero.

The vector $\hat{\mathbf{f}} - \hat{\mathbf{f}}^{(-k)}$ is the difference in predictions obtained when fitting to \mathbf{X} , and those obtained when fitting to \mathbf{X} with the k th column set to zero. When the underlying model in \mathbf{X} contains only main effects (4.2) and no structural error is present, we might expect that

$$\hat{\mathbf{f}} - \hat{\mathbf{f}}^{(-k)} \approx \beta_k^* \mathbf{X}_k.$$

To obtain a measure of variable importance, one could look at the ℓ_2 -norm of $\hat{\mathbf{f}} - \hat{\mathbf{f}}^{(-k)}$, for example [Breiman, 2001].

The difference in predictions can be computed relatively easily by considering the $n \times 2^b L$ matrix $\tilde{\mathbf{S}}$ with entries given by $\tilde{S}_{ilc} = \tilde{S}_{i(c+(l-1)2^b)} = X_{i\tilde{H}_{il}} \mathbb{1}_{\{\Psi_{\tilde{H}_{il}} = c\}}$, where

$$\tilde{H}_{il} := \arg \min_{k \in \mathbf{z}_i \setminus H_{il}} \pi_l(k).$$

Thus \tilde{H}_{il} is the variable index in \mathbf{z}_i whose value under permutation π_l is second smallest among $\{\pi_l(k) : k \in \mathbf{z}_i\}$. If $\mathbf{z}_i \setminus H_{il} = \emptyset$, we simply set $\tilde{S}_{il} = 0$. Then

$$\hat{f}_i - \hat{f}_i^{(-k)} = \sum_{l=1}^L \mathbb{1}_{\{H_{il}=k\}} \sum_{c=1}^{2^b} (S_{ilc} - \tilde{S}_{ilc}) \hat{b}_{lc}. \quad (6.1)$$

Note that we only need to store the $n \times L$ matrix \mathbf{H} and $n \times 2^b L$ matrices \mathbf{S} and $\tilde{\mathbf{S}}$ to compute the variable importance for all variables; moreover the latter matrices only have at most nL non-zero entries each.

Interaction effects are not directly visible, but do manifest themselves in the form of a higher variability among $\{\hat{f}_i - \hat{f}_i^{(-k)} : \mathbf{x}_i \approx \mathbf{x}\}$, for any given value of \mathbf{x} , if variable k is involved in an interaction term. In principle, one could attempt to detect this increased variability, but further investigation of this is beyond the scope of the current work.

6.2 Other fitting procedures

Here we have only considered OLS, ridge regression and ℓ_2 -penalised logistic regression as prediction methods after reducing the design matrix. However, it is also conceivable that other fitting procedures could be suitable. In particular, it would be interesting to look at matching pursuit, boosting and the Lasso, for which results in [Tropp, 2004, Bühlmann, 2006, Van De Geer, 2008] could be leveraged. Matching pursuit would have the computational advantage that the entire \mathbf{S} matrix would not need to be held in memory. Instead, one could create the columns during the fitting process. Such an approach may be useful for problems where the dimension of the hashing-matrix, $2^b L$, needs to be very large to achieve a desired predictive accuracy.

7 Discussion

The large-scale sparse data setting presents many new challenges to statisticians that require novel approaches to overcome them. One could summarise the conventional process by which statistical methodology is developed in two stages: first a procedure that is statistically optimal for the data-generating process of interest is sought out; next, one may attempt to produce fast algorithms for the procedure. In the ‘large p , large n ’ we study here, it often makes more sense to consider computational issues alongside, or even before, statistical ones.

The method of b -bit min-wise hashing [Li and König, 2011] is computationally well-suited to large-scale sparse data, and can retain feasibility where other dimension reduction techniques, such as those based on PCA, may fail. Some of its statistical properties, however, are harder to discern immediately.

In this paper we have derived approximation error bounds for b -bit min-wise hashing and through this also provided some insight into the regularisation properties of the resemblance kernel. We were able to show that not only does b -bit min-wise hashing take advantage of sparsity in the design matrix computationally, it is also able to exploit this for improved statistical performance. In particular, the MSPE of regression following dimension reduction by b -bit min-wise hashing is of the form $\sqrt{q/n}\|\beta^*\|_2$ if the data follow a linear model with coefficient vector β^* and q is the average number of non-zero variables for an observation. The linear model can then be well-approximated by the low-dimensional b -bit min-wise hashed data if the norm of $\|\beta^*\|_2$ is low, as occurs, for example if the signal is approximately replicated in distinct blocks of variables.

In addition, we have shown that more complicated models such as interaction models can be fitted by a regression on the hashed data matrix that contains only main effects. Though a larger dimension L of the hashed data may be required than when approximating a main effects model, no further changes are needed to the procedure.

In summary, regression with only main effects on min-wise hashed data can be a very powerful prediction engine in settings with millions of predictors and observations. Moreover, the memory footprint and computational cost of the procedure is such that this can be performed with ease on standard computing equipment. We expect to see more extensions and applications b -bit min-wise hashing and other hashing algorithms in the future.

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8 Appendix

8.1 Approximation error results

We will let q_i be the number of non-zeroes in the i th row of \mathbf{X} and define $\delta_i = q_i/p$. We will assume that $q_i \geq 1$ for all i . For the proofs of results on approximation error in settings with just main effects, we will make use of the following lemma. This lemma formalises the ideas of the discussion at the end of Section 3.2, that the elements of \mathbf{M} behave rather like geometric random variables.

Lemma 10. *There exist random functions $\{g_l(k)\}_{l=1,\dots,L,k=1,\dots,p}$ defined on the same probability space as the permutations $\boldsymbol{\pi}$ with the following properties:*

- (i) *The random variables $\{g_1(k)\}_{k=1,\dots,p}, \dots, \{g_L(k)\}_{k=1,\dots,p}$ are i.i.d. and are independent of $\boldsymbol{\Psi}$.*
- (ii) *The rank of $g_l(k)$ among $g_l(1), \dots, g_l(p)$ taken in increasing order is $\pi_l(k)$.*
- (iii) *Marginally $g_l(k) \sim \text{Geo}(p^{-1})$.*
- (iv) *$G_{il} := \min_{k \in \mathbf{z}_i} g_l(k) = g_l(H_{il}) \sim \text{Geo}(\delta_i)$.*
- (v) *\mathbf{G} and \mathbf{H} are independent.*

Proof. First consider generating permutations $\boldsymbol{\pi}$ in the following way. Let $m \in \mathbb{N}$ and let $\sigma_1^{(m)}, \dots, \sigma_L^{(m)}$ be L i.i.d. random permutations of $\{1, \dots, mp\}$. For $k = 1, \dots, p$, let

$$g_l^{(m)}(k) = \min_{a=0,\dots,m-1} \sigma_l^{(m)}(k + ap).$$

Note that the $g_l^{(m)}(k)$ are all distinct and any ordering of them is equally likely so they define a random permutation of $\{1, \dots, p\}$. Furthermore, for $j = 1, \dots, mp - m + 1$,

$$\mathbb{P}(g_l^{(m)}(k) = j) = \binom{mp-j}{m-1} / \binom{mp}{m} = \frac{1}{p} \left(1 - \frac{1-m^{-1}}{p-m^{-1}}\right) \cdots \left(1 - \frac{1-m^{-1}}{p-(j-1)m^{-1}}\right).$$

Thus

$$\mathbb{P}(g_l^{(m)}(k) = j) \rightarrow \frac{1}{p} \left(1 - \frac{1}{p}\right)^{j-1}$$

as $m \rightarrow \infty$ for $j = 1, 2, \dots$. Similarly $G_{il}^{(m)} := \min_{k \in \mathbf{z}_i} g_l^{(m)}(k)$ has $\mathbb{P}(G_{il}^{(m)} = j) \rightarrow \delta_i(1 - \delta_i)^{j-1}$ as $m \rightarrow \infty$. Note that $\mathbf{G}^{(m)}$ and \mathbf{H} are independent. Thus

$$\{g_l^{(m)}(k)\}_{l=1,\dots,L,k=1,\dots,p} \xrightarrow{d} \{g_l(k)\}_{l=1,\dots,L,k=1,\dots,p}$$

as $m \rightarrow \infty$ with the random variables $g_l(k)$ having the properties given in the statement of the lemma. \square

In the proofs which follow, we will consider the permutations as having been generated as described by Lemma 10. We will let $\pi = \pi_1$, $M_i = M_{i1}$, $g = g_1$, $G_1 = G_{i1}$, $H_i = H_{i1}$ and $\boldsymbol{\psi} = \boldsymbol{\Psi}_1$. Let $C = 2^b$, $\nu = 2^{-b}$.

The next lemma introduces the general form of \mathbf{b}^* that we will use for the main effects results. It also establishes results on the mean and variance of the approximation and gives a bound on $\mathbb{E}(\|\mathbf{b}^*\|_2^2)$; these will form the basis of the theorems to follow.

Lemma 11. *For a given sequence of weights $\{w_j\}_{j=1}^\infty$, let $\tilde{\mathbf{b}}^* \in \mathbb{R}^{LC}$ be given by*

$$\tilde{b}_{lc}^* = \frac{1}{L} \sum_{k=1}^p \beta_k^* \frac{\mathbb{1}_{\{\Psi_{lk}=c\}} - \nu}{1 - \nu} w_{g_l(k)}$$

and let $\mathbf{b}^* = \mathbb{E}(\tilde{\mathbf{b}}^* | \boldsymbol{\pi})$. We have the following.

(i)

$$\mathbb{E}_{\boldsymbol{\pi}, \boldsymbol{\Psi}}(\mathbf{s}_i^T \mathbf{b}^*) = \frac{1}{p} \mathbf{x}_i^T \boldsymbol{\beta}^* \sum_{\ell=1}^{\infty} (1 - \delta_i)^{\ell-1} w_\ell.$$

(ii)

$$\mathbb{E}_{\boldsymbol{\pi}, \boldsymbol{\Psi}}(\|\mathbf{b}^*\|_2^2) \leq \frac{1}{pL(1 - \nu)} \|\boldsymbol{\beta}^*\|_2^2 \sum_{\ell=1}^{\infty} w_\ell^2. \quad (8.1)$$

(iii)

$$\text{Var}_{\boldsymbol{\pi}, \boldsymbol{\Psi}}(\mathbf{s}_i^T \mathbf{b}^*) \leq \frac{1}{pL(1 - \nu)} \left(\nu \|\boldsymbol{\beta}^*\|_2^2 + (1 - 2\nu) \sum_{k=1}^p X_{ik}^2 \beta_k^{*2} \right) \sum_{\ell=1}^{\infty} w_\ell^2. \quad (8.2)$$

Proof. First note that

$$\mathbb{E} \left(\frac{\mathbb{1}_{\{\psi_k = \psi_j\}} - \nu}{1 - \nu} \middle| \psi_j \right) = \begin{cases} 1 & \text{if } k = j \\ 0 & \text{otherwise} \end{cases} \quad (8.3)$$

$$\mathbb{E} \left(\frac{\mathbb{1}_{\{\psi_k = \psi_j\}} - \nu}{1 - \nu} \frac{\mathbb{1}_{\{\psi_\ell = \psi_j\}} - \nu}{1 - \nu} \middle| \psi_j \right) = \begin{cases} 1 & \text{if } k = \ell = j \\ 0 & \text{if } k \neq \ell \\ \frac{\nu}{1 - \nu} & \text{otherwise.} \end{cases} \quad (8.4)$$

For (i), we have

$$\begin{aligned} \mathbb{E}_{\boldsymbol{\pi}, \boldsymbol{\Psi}}(\mathbf{s}_i^T \mathbf{b}^*) &= \mathbb{E}_{g, \boldsymbol{\psi}} \left(\sum_{c=1}^C \sum_{j=1}^p X_{ij} \mathbb{1}_{\{H_i=j\}} \mathbb{1}_{\{\psi_j=c\}} \sum_{k=1}^p \beta_k^* \frac{\mathbb{1}_{\{\psi_k=c\}} - \nu}{1 - \nu} w_{g(k)} \right) \\ &= \mathbb{E}_g \left(\sum_{k=1}^p X_{ik} \mathbb{1}_{\{H_i=k\}} \beta_k^* w_{g(k)} \right) \\ &= \frac{1}{q_i} \sum_{k=1}^p X_{ik} \beta_k^* \mathbb{E}(w_{G_i}), \end{aligned}$$

where to arrive at the second line we used (8.3).

Turning to (ii), note that each component of \mathbf{b}^* has mean zero and so

$$\mathbb{E}(b_{lc}^*) = \text{Var}(b_{lc}^*) = \text{Var}\{\mathbb{E}(\tilde{b}_{lc}^* | \boldsymbol{\pi})\} \leq \text{Var}(\tilde{b}_{lc}^*).$$

Now we have

$$\mathbb{E}_{g_1, \dots, g_L, \Psi} \|\tilde{\mathbf{b}}^*\|_2^2 = \frac{1}{L} \sum_{c=1}^C \sum_{k, \ell} \beta_k^* \beta_\ell^* \mathbb{E} \left(\frac{\mathbb{1}_{\{\psi_k=c\}} - \nu}{1-\nu} \frac{\mathbb{1}_{\{\psi_\ell=c\}} - \nu}{1-\nu} \right) \mathbb{E}(w_{g(k)} w_{g(\ell)})$$

Using (8.4), we get

$$\mathbb{E}_{g_1, \dots, g_L, \Psi} \|\tilde{\mathbf{b}}^*\|_2^2 = \frac{1}{L(1-\nu)} \sum_k \beta_k^{*2} \mathbb{E}(w_{g(k)}^2) \leq \frac{1}{pL(1-\nu)} \|\boldsymbol{\beta}^*\|_2^2 \sum_{\ell=1}^{\infty} w_\ell^2.$$

For (iii) we argue as follows.

$$\begin{aligned} \text{Var}(\mathbf{s}_i^T \mathbf{b}^*) &\leq \text{Var}(\mathbf{s}_i^T \tilde{\mathbf{b}}^*) \\ &\leq \frac{1}{L} \mathbb{E}_{g, \psi} \left(X_{iH_i}^2 \sum_{k, \ell} \beta_k^* \beta_\ell^* \frac{\mathbb{1}_{\{\psi_k=\psi_{H_i}\}} - \nu}{1-\nu} \frac{\mathbb{1}_{\{\psi_\ell=\psi_{H_i}\}} - \nu}{1-\nu} w_{g(k)} w_{g(\ell)} \right) \end{aligned}$$

Using (8.4) and the fact that $\mathbf{X} \in [-1, 1]^n$ *timesp*, we have

$$\begin{aligned} \text{Var}(\mathbf{s}_i^T \mathbf{b}^*) &\leq \frac{1}{L} \mathbb{E} \left\{ X_{iH_i}^2 \left(\frac{\nu}{1-\nu} \sum_{k=1}^p (\beta_k^*)^2 w_{g(k)}^2 + \frac{1-2\nu}{1-\nu} (\beta_{H_i}^*)^2 w_{G_i}^2 \right) \right\} \\ &\leq \frac{1}{L(1-\nu)} \left\{ \nu \sum_{k=1}^p \beta_k^{*2} \mathbb{E}(w_{g(k)}^2) + \frac{1-2\nu}{q_i} \mathbb{E}(w_{G_i}^2) \sum_{k=1}^p X_{ik}^2 \beta_k^{*2} \right\}. \end{aligned} \quad (8.5)$$

The result then follows as

$$\sum_{\ell=1}^{\infty} w_\ell^2 \geq \mathbb{E}(w_{g(k)}^2) = \frac{1}{p} \sum_{\ell=1}^{\infty} w_\ell^2 \left(1 - \frac{1}{p}\right)^{\ell-1} \geq \frac{\delta_i}{q_i} \sum_{\ell=1}^{\infty} w_\ell^2 (1 - \delta_i)^{\ell-1} = \frac{\mathbb{E}(w_{G_i}^2)}{q_i}. \quad \square$$

Proof of Theorem 1

We use a \mathbf{b}^* and $\tilde{\mathbf{b}}^*$ as in Lemma 11 but here we choose the weights w_ℓ so as to minimise $\sum_{\ell=1}^{\infty} w_\ell^2$ (a term which features in our upper bounds on the variance and $\mathbb{E}(\|\mathbf{b}^*\|_2^2)$) subject to the unbiasedness constraint (i). The unbiasedness constraint amounts to

$$\sum_{\ell=1}^{\infty} (1-\delta)^{\ell-1} w_\ell = p.$$

Performing the minimisation with this constraint yields

$$w_\ell = p \frac{(1-\delta)^{\ell-1}}{\sum_{\ell=1}^{\infty} (1-\delta)^{2\ell-2}}.$$

With this choice we have

$$\sum_{\ell=1}^{\infty} w_\ell^2 = p^2 \left(\sum_{\ell=1}^{\infty} (1-\delta)^{2\ell-2} \right)^{-1} = p^2 \{1 - (1-\delta)^2\} = (2-\delta)qp.$$

Substituting into (8.1) and (8.2) then yields the result. \square

Proof of Theorem 2

We use a \mathbf{b}^* and $\tilde{\mathbf{b}}^*$ as in Lemma 11 but here we take

$$w_{\ell+1} = p(-1)^\ell \frac{\kappa^{(\ell)}(1)}{\ell!} \{ \mathbb{1}_{\{\ell \leq \lfloor m \rfloor\}} + (m - \lfloor m \rfloor) \mathbb{1}_{\{\ell = \lceil m \rceil\}} \}$$

where $m > 0$ is a parameter to be chosen. Thus the weights correspond to coefficients from a truncated Taylor series expansion of κ about 1. We have

$$\mathbb{E}_{\pi, \Psi} [\{ (\delta_{\min}/\delta_i)^a \mathbf{x}_i^T \boldsymbol{\beta}^* - \mathbf{s}_i^T \mathbf{b}^* \}^2] = \{ (\delta_{\min}/\delta_i)^a \mathbf{x}_i^T \boldsymbol{\beta}^* - \mathbb{E}_{\pi, \Psi} (\mathbf{s}_i^T \mathbf{b}^*) \}^2 + \text{Var}_{\pi, \Psi} (\mathbf{s}_i^T \mathbf{b}^*).$$

We first bound the variance term by bounding the squared sum of the sequence of weights. To this end, we note that by Lemma 18

$$\frac{\delta_{\min}^{-2a}}{p^2} \sum_{\ell=1}^{\infty} w_\ell^2 \leq 1 + a^2 + a^2 e^{2a} \left(\sum_{\ell=2}^{\lfloor m \rfloor} \frac{1}{\ell^{2(1-a)}} + \frac{m - \lfloor m \rfloor}{\lceil m \rceil^{2(1-a)}} \right).$$

Now

$$\begin{aligned} \sum_{\ell=2}^{\lfloor m \rfloor} \frac{1}{\ell^{2(1-a)}} + \frac{m - \lfloor m \rfloor}{\lceil m \rceil^{2(1-a)}} &\leq \int_1^m \frac{1}{\ell^{2(a-1)}} d\ell \\ &= \begin{cases} \frac{m^{2a-1} - 1}{2a-1} & \text{if } a \neq 1/2 \\ \log(m) & \text{if } a = 1/2. \end{cases} \end{aligned}$$

Let

$$\tau_a(m) = \begin{cases} e \log(me^{5/e})/4 & \text{if } a = 1/2, \\ a^2 e^{2a} m^{2a-1} / (2a-1) & \text{if } 1/2 < a \leq 1. \end{cases}$$

Then

$$\sum_{\ell=1}^{\infty} w_\ell^2 \leq p^2 \delta_{\min}^{2a} \tau_a(m). \quad (8.6)$$

The variance is then at most

$$\delta_{\min}^{2a} \tau_a(m) \frac{p}{L(1-\nu)} \left(\nu \|\boldsymbol{\beta}^*\|_2^2 + (1-2\nu) \sum_{k=1}^p X_{ik}^2 \beta_k^{*2} \right).$$

Turning now to the bias term, note first that by (i) of Lemma 11, this is equal to

$$(\mathbf{x}_i^T \boldsymbol{\beta}^*)^2 \left\{ (\delta_{\min}/\delta_i)^a - \frac{1}{p} \sum_{\ell=1}^{\infty} (1-\delta_i)^{\ell-1} w_\ell \right\}^2. \quad (8.7)$$

We see this is bounded above by

$$\delta_{\min}^{2a} (\mathbf{x}_i^T \boldsymbol{\beta}^*)^2 \left\{ a e^a \left(\sum_{\ell=\lceil m \rceil}^{\infty} (1-\delta_i)^\ell \frac{1}{\ell^{1-a}} \right) \right\}^2.$$

Now

$$\sum_{\ell=\lceil m \rceil}^{\infty} (1 - \delta_i)^\ell \frac{1}{\ell^{1-a}} \leq \frac{e^{-\delta_i m}}{m^{1-a} \delta_i}.$$

By the Cauchy–Schwarz inequality (assuming $X_{ij} \in [-1, 1]$)

$$\frac{(\mathbf{x}_i^T \boldsymbol{\beta}^*)^2}{\delta_i} = \frac{1}{\delta_i} \left(\sum_{k \in \mathbf{z}_i} X_{ik} \beta_k^* \right)^2 \leq p \sum_{k=1}^p X_{ik}^2 \beta_k^{*2} \leq p \|\boldsymbol{\beta}^*\|_2^2.$$

Thus the squared bias is at most

$$\frac{p}{1 - \nu} \frac{a^2 e^{2a}}{m^{1-2a}} \max_{i=1, \dots, n} \left(\frac{e^{-2\delta_i m}}{m \delta_i} \right) \left(\nu \|\boldsymbol{\beta}^*\|_2^2 + (1 - 2\nu) \sum_{k=1}^p X_{ik}^2 \beta_k^{*2} \right).$$

Therefore the MSE (now averaging over the observations) is bounded by the minimum over $m > 0$ of

$$\frac{p}{L(1 - 2^{-b})} \delta_{\min}^{2a} \left\{ \tau_a(m) + \frac{a^2 e^{2a}}{m^{1-2a}} \max_{i=1, \dots, n} \left(\frac{e^{-2\delta_i m}}{m \delta_i} \right) \right\} \|\boldsymbol{\beta}^*\|_2^2.$$

For $a = 1/2$, we set $m = \log(L)/\{2\delta_{\min}\}$. This yields

$$\begin{aligned} \min_{m>0} \left\{ \tau_{1/2}(m) + \frac{Le}{4} \max_{i=1, \dots, n} \left(\frac{e^{-2\delta_i m}}{m \delta_i} \right) \right\} &\leq \frac{e}{4} \left\{ \log \left(\frac{\log(L) e^{5/e}}{2\delta_{\min}} \right) + \frac{2}{\log(L)} \right\} \\ &\leq \log\{4 \log(L)/\delta_{\min}\} \end{aligned}$$

provided $L \geq 10$ and $\delta_{\min} \leq 1/2$. Finally the bound for $a > 1/2$ comes from setting

$$m = \frac{1}{2} \log\{2(2a - 1)L\}/\delta_{\min}$$

which gives

$$\begin{aligned} \min_{m>0} \left\{ \tau_a(m) + \frac{La^2 e^{2a}}{m^{1-2a}} \max_{i=1, \dots, n} \left(\frac{e^{-2\delta_i m}}{m \delta_i} \right) \right\} &\leq \frac{\delta_{\min}^{1-2a} a^2 e^{2a}}{2^{2a-1} (2a - 1)} [\log\{2(2a - 1)L\}]^{2a-2} \log\{2(2a - 1)eL\} \\ &\leq \frac{4\delta_{\min}^{1-2a}}{1 - 2a} [\log\{2(2a - 1)L\}]^{2a-1} \end{aligned}$$

for $L \geq 2/(1 - 2a)$. Using the bounds on τ_a with these choices of m and (8.6), we obtain the bounds on $\mathbb{E}(\|\mathbf{b}^*\|_2^2)$ by substituting into (8.1). \square

8.1.1 Unequal row sparsity and constant row-scaling

Here we prove results indicated after the presentation of Theorem 1 in Section 3.1. When the scaling function is simply the constant 1, the spread of the δ_i becomes more critical in determining how well the signal can be approximated. Define

$$\begin{aligned} \bar{\delta} &= \frac{1}{n} \sum_{i=1}^n \delta_i, \\ \mathcal{V}(\boldsymbol{\delta}) &= \frac{1}{\|\mathbf{X}\boldsymbol{\beta}^*\|_2^2} \sum_{i=1}^n (\mathbf{x}_i^T \boldsymbol{\beta}^*)^2 (\delta_i - \bar{\delta})^2. \end{aligned}$$

Theorem 12. *Suppose*

$$2^b L(1 - 2^{-b}) \leq \frac{p(2\bar{\delta})^3 \|\boldsymbol{\beta}^*\|_b^2}{\|\mathbf{X}\boldsymbol{\beta}^*\|_2^2 \mathcal{V}(\boldsymbol{\delta})/n}. \quad (8.8)$$

Then there exists $\mathbf{b}^* \in \mathbb{R}^L$ such that the approximation error satisfies

$$\frac{1}{n} \mathbb{E}_{\boldsymbol{\pi}, \boldsymbol{\Psi}} \{ \|\mathbf{X}\boldsymbol{\beta}^* - \mathbf{S}\mathbf{b}^*\|_2^2 \} \leq \frac{6p\bar{\delta}}{2^b L(1 - 2^{-b})} \|\boldsymbol{\beta}^*\|_b^2, \quad (8.9)$$

and

$$\mathbb{E}_{\boldsymbol{\pi}, \boldsymbol{\Psi}} (\|\mathbf{b}^*\|_2^2) \leq \frac{2\bar{q}}{L(1 - 2^{-b})} \|\boldsymbol{\beta}^*\|_2^2. \quad (8.10)$$

Provided $2^b L$ is not too large, we recover essentially the same approximation error bound as Theorem 1 up to a constant factor, but with the row sparsity replaced by the average row sparsity $\bar{\delta}$. In the simple situation where the entries of \mathbf{X} are realisations of i.i.d. Bernoulli random variables with probability δ , we would have $\bar{\delta} \approx \delta$, $\|\mathbf{X}\boldsymbol{\beta}^*\|_2^2/n \approx \delta \|\boldsymbol{\beta}^*\|_2^2$ and $\mathcal{V}(\boldsymbol{\delta}) \approx \delta/p$. Substituting these values into the requirement on $2^b L$ shows that the condition reduces to $2^b L \leq 8p^2 \delta \{1 + (2^b - 2)\delta\}$. Note that typically one would choose $2^b L$ of the order $\bar{\delta}p$. More generally, provided $\mathcal{V}(\boldsymbol{\delta})$ and $\|\mathbf{X}\boldsymbol{\beta}^*\|_2^2/\|\boldsymbol{\beta}^*\|_2^2$ are small, we can expect that the bound of Theorem 1 will hold true, up to a constant factor.

Proof of Theorem 12

We use a \mathbf{b}^* and $\tilde{\mathbf{b}}^*$ as in Lemma 11 taking

$$w_\ell = p(1 - \bar{\delta})^{\ell-1} \mathbb{1}_{\{\ell \leq m\}} \frac{\bar{\delta}(2 - \bar{\delta})}{1 - (1 - \bar{\delta})^{2m}}.$$

where $m \in \mathbb{N}$ is a parameter to be chosen. This gives

$$\frac{1}{p^2} \sum_{\ell=1}^{\infty} w_\ell^2 = \frac{\bar{\delta}(2 - \bar{\delta})}{1 - (1 - \bar{\delta})^{2m}},$$

which gives us a bound on the variance term.

Lemma 11 (i) gives the expression for the bias term. To bound this, first note that

$$\frac{1}{p} \sum_{\ell=1}^m (1 - \bar{\delta})^{\ell-1} w_\ell = 1.$$

Next

$$\begin{aligned} \left[\sum_{\ell=1}^m (1 - \bar{\delta})^{\ell-1} \{ (1 - \bar{\delta})^{\ell-1} - (1 - \delta_i)^{\ell-1} \} \right]^2 &= (\delta_i - \bar{\delta})^2 \left[\sum_{\ell=1}^m (1 - \bar{\delta})^{\ell-1} \sum_{k=0}^{\ell-2} (1 - \bar{\delta})^k (1 - \delta_i)^{\ell-2-k} \right]^2 \\ &\leq (\delta_i - \bar{\delta})^2 \left(\sum_{\ell=1}^m (1 - \bar{\delta})^{\ell-1} (\ell - 1) \right)^2 \\ &= \min \left\{ \frac{m(m-1)}{2}, \frac{1}{\bar{\delta}^2} \right\}^2 (\delta_i - \bar{\delta})^2. \end{aligned}$$

Also note that as

$$(1 - \bar{\delta})^{2m} \leq 1 - 2m\bar{\delta} + m(2m - 1)\bar{\delta}^2$$

we have

$$\begin{aligned} \frac{\bar{\delta}(2 - \bar{\delta})}{1 - (1 - \bar{\delta})^{2m}} &\leq \frac{2}{2m - m(2m - 1)\bar{\delta}} \mathbb{1}_{\{m \leq 1/(2\bar{\delta})\}} + \frac{2}{1/\bar{\delta} - (1/\bar{\delta} - 1)/2} \mathbb{1}_{\{m > 1/(2\bar{\delta})\}} \\ &\leq \max\left(\frac{2}{m + 1/2}, \frac{4\bar{\delta}}{1 + \bar{\delta}}\right) \end{aligned}$$

and for $m \leq 1/(2\bar{\delta}) + 1/2$,

$$\frac{m(m - 1)}{2} \max\left(\frac{2}{m + 1/2}, \frac{4\bar{\delta}}{1 + \bar{\delta}}\right) \leq (m - 1/2) \mathbb{1}_{\{1 < m \leq 1/(2\bar{\delta}) + 1/2\}}.$$

Thus the overall approximation error is bounded above by the minimum over $m = 1, 2, \dots, \lfloor 1/(2\bar{\delta}) + 1/2 \rfloor$ of

$$\mathbb{1}_{\{m > 1\}} (m - 1/2)^2 \frac{1}{n} \|\mathbf{X}\boldsymbol{\beta}^*\|_2^2 \mathcal{V}(\boldsymbol{\delta}) + \max\left(\frac{2}{m + 1/2}, 4\bar{\delta}\right) \frac{p}{2^b L(1 - 2^{-b})} \|\boldsymbol{\beta}^*\|_b^2,$$

which in turn is bounded by the minimum over $m \in [0, 1/(2\bar{\delta})]$ of

$$m^2 \frac{1}{n} \|\mathbf{X}\boldsymbol{\beta}^*\|_2^2 \mathcal{V}(\boldsymbol{\delta}) + \frac{2}{m} \frac{p}{2^b L(1 - 2^{-b})} \|\boldsymbol{\beta}^*\|_b^2. \quad (8.11)$$

Optimising over $m > 0$ in the above then gives

$$m = \min\left\{\left(\frac{p \|\boldsymbol{\beta}^*\|_b^2}{2^b L(1 - 2^{-b}) \|\mathbf{X}\boldsymbol{\beta}^*\|_2^2 \mathcal{V}(\boldsymbol{\delta}) / n}\right)^{1/3}, \frac{1}{2\bar{\delta}}\right\}.$$

The condition on L (8.8) ensures that the minimum is achieved at $1/(2\bar{\delta})$. Substituting this value of m into (8.11) then gives (8.9). For (8.10) we note that

$$\sum_{\ell=1}^{\infty} w_{\ell}^2 \leq 2p^2 \bar{\delta},$$

and use Lemma 11 (ii). □

Proof of Theorem 6

We let $\mathbf{b}^* = \mathbf{b}^{*,(1)} + \mathbf{b}^{*,(2)}$ where $\mathbf{b}^{*,(1)}$ is chosen in line with Theorem 1. Explicitly, let $\mathbf{b}^{*,(1)} = \mathbb{E}(\tilde{\mathbf{b}}^* | \boldsymbol{\pi})$ where

$$\tilde{b}_{lc}^* = \frac{p}{L} \sum_{k=1}^p \theta_k^{*,(1)} \frac{\mathbb{1}_{\{\Psi_{lk}=c\}} - \nu}{1 - \nu} \frac{(1 - \delta)^{g_l(k) - 1}}{\sum_{\ell=1}^{\infty} (1 - \delta)^{2\ell - 2}}.$$

We construct $\mathbf{b}^{*,(2)}$ to approximate the interactions as follows. Let

$$b_{lc}^{*,(2)} = \frac{pq}{L} \sum_{k=1}^p \frac{\mathbb{1}_{\{\Psi_{lk}=c\}} - \nu}{1 - \nu} \sum_{k_1=1}^p \Theta_{kk_1}^{*,(2)} \mathbb{1}_{\{\pi_l(k_1) < \pi_l(k)\}} w_{\pi_l(k)},$$

where $\mathbf{w} \in \mathbb{R}^p$ is a vector of weights to be chosen such that

$$\mathbb{E}_{\boldsymbol{\pi}, \boldsymbol{\Psi}}(\mathbf{s}_i^T \mathbf{b}^{*,(2)}) = \sum_{k, k_1} X_{ik} \mathbb{1}_{\{X_{ik_1}=0\}} \Theta_{kk_1}^{*,(2)}. \quad (8.12)$$

We compute

$$\begin{aligned} \mathbb{E}_{\boldsymbol{\pi}, \boldsymbol{\Psi}}(\mathbf{s}_i^T \mathbf{b}^{*,(2)}) &= \frac{pq}{L} \sum_{l=1}^L \sum_{c=1}^C \mathbb{E}_{\boldsymbol{\pi}_l, \boldsymbol{\Psi}_l} \left(S_{ilc} \sum_{k=1}^p \frac{\mathbb{1}_{\{\Psi_{kl}=c\}} - \nu}{1 - \nu} \sum_{k_1=1}^p \Theta_{kk_1}^{*,(2)} \mathbb{1}_{\{\pi_l(k_1) < \pi_l(k)\}} w_{\pi_l(k)} \right) \\ &= pq \mathbb{E}_{\boldsymbol{\pi}, \boldsymbol{\psi}} \left(\sum_{c=1}^C \sum_{j=1}^p X_{ij} \mathbb{1}_{\{H_i=j\}} \mathbb{1}_{\{\psi_j=c\}} \sum_{k=1}^p \frac{\mathbb{1}_{\{\psi_k=c\}} - \nu}{1 - \nu} \sum_{k_1=1}^p \Theta_{kk_1}^{*,(2)} \mathbb{1}_{\{\pi(k_1) < \pi(k)\}} w_{\pi(k)} \right) \\ &= pq \mathbb{E}_{\boldsymbol{\pi}} \left(\sum_{k=1}^p X_{ik} \mathbb{1}_{\{H_i=k\}} \sum_{k_1=1}^p \Theta_{kk_1}^{*,(2)} \mathbb{1}_{\{\pi(k_1) < \pi(k)\}} \sum_{\ell=2}^p w_{\ell} \mathbb{1}_{\{\pi(k)=\ell\}} \right). \end{aligned}$$

where in the final line we have appealed to (8.3). Now observe that for $k \in \mathbf{z}_i$,

$$\mathbb{1}_{\{H_i=k\}} \mathbb{1}_{\{\pi(k_1) < \pi(k)\}} \mathbb{1}_{\{\pi(k)=\ell\}} = \mathbb{1}_{\{X_{ik_1}=0\}} \mathbb{1}_{\{H_i=k\}} \mathbb{1}_{\{M_i=\ell, \pi(k_1) < \ell\}},$$

and $\mathbb{1}_{\{H_i=k\}}$ and $\mathbb{1}_{\{M_i=\ell, \pi(k_1) < \ell\}}$ are independent. Thus we have

$$\begin{aligned} \mathbb{E}_{\boldsymbol{\pi}, \boldsymbol{\Psi}}((\mathbf{Sb}^{*,(2)})_i) &= \sum_{k, k_1} X_{ik} \mathbb{1}_{\{X_{ik_1}=0\}} \Theta_{kk_1}^{*,(2)} \sum_{\ell=1}^p p \mathbb{P}_{\boldsymbol{\pi}}(M_i = \ell, \pi(k_1) < \ell) w_{\ell} \\ &= \sum_{k, k_1} X_{ik} \mathbb{1}_{\{X_{ik_1}=0\}} \Theta_{kk_1}^{*,(2)} \sum_{\ell=2}^p (\ell - 1) \mathbb{P}_{\boldsymbol{\pi}}(M_i = \ell | \pi(k_1) < \ell) w_{\ell} \\ &= \sum_{k, k_1} X_{ik} \mathbb{1}_{\{X_{ik_1}=0\}} \Theta_{kk_1}^{*,(2)} \sum_{\ell=2}^p (\ell - 1) \frac{\binom{p-\ell}{q-1}}{\binom{p-1}{q}} w_{\ell}. \end{aligned}$$

Thus if we choose \mathbf{w} such that

$$\sum_{\ell=2}^p (\ell - 1) \frac{\binom{p-\ell}{q-1}}{\binom{p-1}{q}} w_{\ell} = 1, \quad (8.13)$$

property (8.12) will be satisfied.

Next we compute

$$\begin{aligned}
\mathbb{E}(\|\mathbf{b}^{*,(2)}\|_2^2) &\leq \frac{p^2 q^2}{L(1-\nu)} \sum_{k=1}^p \mathbb{E} \left\{ \left(\sum_{k_1=1}^p \Theta_{kk_1}^{*,(2)} \mathbb{1}_{\{\pi(k_1) < \pi(k)\}} \right)^2 w_{\pi(k)}^2 \right\} \\
&= \frac{p^2 q^2}{L(1-\nu)} \sum_{k=1}^p \sum_{\ell=1}^p w_\ell^2 \left(\sum_{k_1} (\Theta_{kk_1}^{*,(2)})^2 \mathbb{P}(\pi(k) = \ell, \pi(k_1) < \ell) \right. \\
&\quad \left. + \sum_{k_1 \neq k_2} \Theta_{kk_1}^{*,(2)} \Theta_{kk_2}^{*,(2)} \mathbb{P}(\pi(k) = \ell, \pi(k_1) < \ell, \pi(k_2) < \ell) \right) \\
&= \frac{pq^2}{L(1-\nu)} \sum_{k=1}^p \sum_{\ell=2}^p w_\ell^2 \left(\frac{\ell-1}{p-1} \sum_{k_1} (\Theta_{kk_1}^{*,(2)})^2 + \frac{(\ell-1)(\ell-2)}{(p-1)(p-2)} \sum_{k_1 \neq k_2} \Theta_{kk_1}^{*,(2)} \Theta_{kk_2}^{*,(2)} \right) \\
&\leq \frac{pq^2}{(p-1)L(1-\nu)} \sum_{k, k_1, k_2} \left| \Theta_{kk_1}^{*,(2)} \Theta_{kk_2}^{*,(2)} \right| \sum_{\ell=2}^p (\ell-1) w_\ell^2. \tag{8.14}
\end{aligned}$$

Choosing

$$w_\ell = \frac{\binom{p-\ell}{q-1} / \binom{p-1}{q}}{\sum_{\ell'=2}^p (\ell'-1) \left\{ \binom{p-\ell'}{q-1} / \binom{p-1}{q} \right\}^2} \tag{8.15}$$

minimises (8.14) subject to (8.13) to give

$$\mathbb{E}_{\boldsymbol{\pi}, \boldsymbol{\Psi}}(\|\mathbf{b}^{*,(2)}\|_2^2) \leq \frac{pq^2}{(p-1)L(1-\nu)} \sum_{k, k_1, k_2} \left| \Theta_{kk_1}^{*,(2)} \Theta_{kk_2}^{*,(2)} \right| \left\{ \sum_{\ell=1}^{p-1} \ell \left(\frac{\binom{p-1-\ell}{q-1}}{\binom{p-1}{q}} \right)^2 \right\}^{-1}.$$

Finally, Lemma 17 bounds the right-most term from above to yield

$$\mathbb{E}_{\boldsymbol{\pi}, \boldsymbol{\Psi}}(\|\mathbf{b}^{*,(2)}\|_2^2) \leq \frac{2\{(2-\delta)q\}^2}{L(1-\nu)} \sum_{k, k_1, k_2} \left| \Theta_{kk_1}^{*,(2)} \Theta_{kk_2}^{*,(2)} \right|. \tag{8.16}$$

Now we turn to the mean-squared error. Observe that $\mathbf{s}_i^T \mathbf{b}^*$ is a sum of L independent random variables, each having the same distribution as

$$\sum_{c=1}^C S_{i1c} b_{1c}^* = \sum_{c=1}^C S_{i1c} (b_{1c}^{*,(1)} + b_{1c}^{*,(2)}).$$

Thus

$$\begin{aligned}
\text{Var}(\mathbf{s}_i^T \mathbf{b}^*) &\leq \frac{1}{L} \mathbb{E} \left(\sum_{c=1}^C S_{i1c} (b_{1c}^{*,(1)} + b_{1c}^{*,(2)}) \right)^2 \\
&\leq \frac{1}{L} \left[\left\{ \mathbb{E} \left(\sum_{c=1}^C S_{i1c} b_{1c}^{*,(1)} \right)^2 \right\}^{1/2} + \left\{ \mathbb{E} \left(\sum_{c=1}^C S_{i1c} b_{1c}^{*,(2)} \right)^2 \right\}^{1/2} \right]^2,
\end{aligned}$$

where we have used the Cauchy–Schwarz inequality in the final line. Now using the fact that $\|\mathbf{X}\|_\infty \leq 1$, and following the argument that leads to (8.5), we arrive at

$$\begin{aligned} \mathbb{E} \left(\sum_{c=1}^C S_{i1c} \mathbf{b}_{1c}^{*,(2)} \right)^2 &= p^2 q^2 \mathbb{E} \left\{ \frac{\nu}{1-\nu} \sum_{k=1}^p \left(\sum_{k_1=1}^p \Theta_{kk_1}^{*,(2)} \mathbb{1}_{\{\pi(k_1) < \pi(k)\}} w_{\pi(k)} \right)^2 \right. \\ &\quad \left. + \frac{1-2\nu}{1-\nu} X_{iH_i}^2 \left(\sum_{k_1=1}^p \Theta_{H_i k_1}^{*,(2)} \mathbb{1}_{\{\pi(k_1) < M_i\}} w_{M_i} \right)^2 \right\}. \end{aligned} \quad (8.17)$$

We have

$$\begin{aligned} \mathbb{E} \left\{ X_{iH_i}^2 \left(\sum_{k_1=1}^p \Theta_{H_i k_1}^{*,(2)} \mathbb{1}_{\{\pi(k_1) < M_i\}} w_{M_i} \right)^2 \right\} &= \frac{1}{q} \sum_{k=1}^p \sum_{\ell=1}^p X_{ik}^2 \mathbb{E} \left\{ \left(\sum_{k_1} \Theta_{k,k_1}^{*,(2)} \mathbb{1}_{\{\pi(k_1) < \ell\}} w_\ell \right)^2 \mathbb{1}_{\{M_i = \ell\}} \right\} \\ &= \sum_{k=1}^p X_{ik}^2 \sum_{\ell=2}^p w_\ell^2 \left(\sum_{k_1} (\Theta_{kk_1}^{*,(2)})^2 \mathbb{P}(M_i = \ell, \pi(k_1) < \ell) + \sum_{k_1 \neq k_2} \Theta_{kk_1}^{*,(2)} \Theta_{kk_2}^{*,(2)} \mathbb{P}(M_i = \ell, \pi(k_1) < \ell, \pi(k_2) < \ell) \right) \\ &= \sum_{k=1}^p X_{ik}^2 \sum_{\ell=2}^p w_\ell^2 \left(\frac{\ell-1}{p-1} \frac{\binom{p-\ell}{q-1}}{\binom{p-1}{q}} \sum_{k_1} (\Theta_{kk_1}^{*,(2)})^2 + \frac{(\ell-1)(\ell-2)}{(p-1)(p-2)} \frac{\binom{p-\ell}{q-1}}{\binom{p-2}{q}} \sum_{k_1 \neq k_2} \Theta_{kk_1}^{*,(2)} \Theta_{kk_2}^{*,(2)} \right). \end{aligned} \quad (8.18)$$

Now

$$\frac{\binom{p-\ell}{q-1}}{\binom{p-1}{q}} \leq \frac{q}{p-1} \quad \text{and} \quad \frac{\ell-2}{p-2} \frac{\binom{p-\ell}{q-1}}{\binom{p-2}{q}} \leq \frac{q}{p-1}.$$

Thus by Lemma 17 the quantity in (8.18) is at most

$$\frac{2(2-\delta)^2 \delta}{p^2} \sum_{k, k_1, k_2} \left| X_{ik}^2 \Theta_{kk_1}^{*,(2)} \Theta_{kk_2}^{*,(2)} \right|.$$

Returning to (8.17) and using the argument leading to (8.14) therefore gives us

$$\mathbb{E} \left(\sum_{c=1}^C S_{i1c} \mathbf{b}_{1c}^{*,(2)} \right)^2 \leq 2(2-\delta)^2 q^2 \left(\frac{\nu}{1-\nu} \sum_{k, k_1, k_2} \left| \Theta_{kk_1}^{*,(2)} \Theta_{kk_2}^{*,(2)} \right| + \delta \frac{1-2\nu}{1-\nu} \sum_{k, k_1, k_2} \left| X_{ik}^2 \Theta_{kk_1}^{*,(2)} \Theta_{kk_2}^{*,(2)} \right| \right),$$

which then gives part (iii) of the result. \square

8.2 Prediction error results

Here we prove results for the prediction error under linear and logistic regression models. We denote the signal to be estimated by \mathbf{f}^* and assume the existence of a $\mathbf{b}^* \in \mathbb{R}^{2^b L}$ with

$$\begin{aligned} \frac{1}{n} \mathbb{E}(\|\mathbf{f}^* - \mathbf{S}\mathbf{b}^*\|_2^2) &\leq c_1/L \\ \mathbb{E}(\|\mathbf{b}^*\|_2^2) &\leq c_2/L. \end{aligned}$$

Explicit constructions for such coefficient vectors are provided in the previous section. Using the results here in conjunction with the approximation error results proved in Section 8.1 yield Theorems 3–9: for example, substituting (iii) of Theorem 1 immediately gives Theorem 3.

8.2.1 Linear regression

We assume the model

$$\mathbf{Y} = \alpha^* \mathbf{1} + \mathbf{f}^* + \boldsymbol{\varepsilon}, \quad (8.19)$$

where $\text{Var}(\boldsymbol{\varepsilon}) = \sigma^2 \mathbf{I}$ and our goal is to estimate \mathbf{f}^* .

Theorem 13. *Let $(\hat{\alpha}, \hat{\mathbf{b}})$ be the least squares estimator (4.4). Then*

$$\text{MSPE}((\hat{\alpha}, \hat{\mathbf{b}})) \leq \frac{c_1}{L} + \frac{\sigma^2 \{(2^b - 1)L + 1\}}{n}.$$

Proof. Let us write

$$\mathbf{Y} = \alpha^* \mathbf{1} + \mathbf{f}^* + \boldsymbol{\varepsilon} = \alpha^* \mathbf{1} + \mathbf{S}\mathbf{b}^* + \boldsymbol{\Delta} + \boldsymbol{\varepsilon},$$

so $\boldsymbol{\Delta}$ is the approximation error of $\mathbf{S}\mathbf{b}^*$. Then we have

$$\text{MSPE}((\hat{\alpha}, \hat{\mathbf{b}})) = \frac{1}{n} \mathbb{E}_{\boldsymbol{\varepsilon}, \boldsymbol{\pi}, \boldsymbol{\Psi}} (\|\alpha^* \mathbf{1} + \mathbf{f}^* - \hat{\alpha} \mathbf{1} - \mathbf{S}\hat{\mathbf{b}}\|_2^2).$$

Now let $\check{\mathbf{S}} = (\mathbf{1} \ \mathbf{S})$, and $\mathbf{P}_{\check{\mathbf{S}}}$ be the projection on to the column space of $\check{\mathbf{S}}$ (so $\mathbf{P}_{\check{\mathbf{S}}} = \check{\mathbf{S}}\check{\mathbf{S}}^+$, where $\check{\mathbf{S}}^+$ denotes the Moore–Penrose pseudoinverse of $\check{\mathbf{S}}$). We have the following decomposition.

$$\begin{aligned} \alpha^* \mathbf{1} + \mathbf{f}^* - \hat{\alpha} \mathbf{1} - \mathbf{S}\hat{\mathbf{b}} &= \alpha^* \mathbf{1} + \mathbf{f}^* - \mathbf{P}_{\check{\mathbf{S}}} \mathbf{Y} \\ &= \alpha^* \mathbf{1} + \mathbf{S}\mathbf{b}^* + \boldsymbol{\Delta} - \mathbf{P}_{\check{\mathbf{S}}}(\alpha^* \mathbf{1} + \mathbf{S}\mathbf{b}^* + \boldsymbol{\Delta} + \boldsymbol{\varepsilon}) \\ &= (\mathbf{I} - \mathbf{P}_{\check{\mathbf{S}}})\boldsymbol{\Delta} - \mathbf{P}_{\check{\mathbf{S}}}\boldsymbol{\varepsilon}. \end{aligned}$$

Hence

$$\begin{aligned} \text{MSPE}((\hat{\alpha}, \hat{\mathbf{b}})) &= \frac{1}{n} \mathbb{E}_{\boldsymbol{\varepsilon}, \boldsymbol{\pi}, \boldsymbol{\Psi}} (\|(\mathbf{I} - \mathbf{P}_{\check{\mathbf{S}}})\boldsymbol{\Delta} - \mathbf{P}_{\check{\mathbf{S}}}\boldsymbol{\varepsilon}\|_2^2) \\ &= \frac{1}{n} \mathbb{E}_{\boldsymbol{\pi}, \boldsymbol{\Psi}} (\|(\mathbf{I} - \mathbf{P}_{\check{\mathbf{S}}})\boldsymbol{\Delta}\|_2^2) + \frac{1}{n} \mathbb{E}_{\boldsymbol{\pi}, \boldsymbol{\Psi}} \{\mathbb{E}_{\boldsymbol{\varepsilon}} (\|\mathbf{P}_{\check{\mathbf{S}}}\boldsymbol{\varepsilon}\|_2^2 \mid \boldsymbol{\pi}, \boldsymbol{\Psi})\} \\ &\leq \frac{1}{n} \mathbb{E}_{\boldsymbol{\pi}, \boldsymbol{\Psi}} (\|\boldsymbol{\Delta}\|_2^2) + \frac{\sigma^2 \{(2^b - 1)L + 1\}}{n} \\ &\leq \frac{c_1}{L} + \frac{\sigma^2 \{(2^b - 1)L + 1\}}{n}, \end{aligned} \quad (8.20)$$

where in for (8.20) we have used the fact that $\text{rank}(\check{\mathbf{S}}) \leq (2^b - 1)L + 1$ as each the L blocks sums to a vector of 1's \square

Theorem 14. *There exists λ depending on \mathbf{f}^* and \mathbf{S} such that defining*

$$(\hat{\alpha}, \hat{\mathbf{b}}) := \arg \min_{(\alpha, \mathbf{b}) \in \mathbb{R} \times \mathbb{R}^L} \|\mathbf{Y} - \alpha \mathbf{1} - \mathbf{S}\mathbf{b}\|_2^2 \quad \text{such that } \|\mathbf{b}\|_2^2 \leq \lambda,$$

we have

$$\text{MSPE}((\hat{\alpha}, \hat{\mathbf{b}})) \leq \sigma \sqrt{\frac{c_2}{n}} + \frac{c_1}{L} + \frac{\sigma^2}{n}.$$

Proof. We will take $\lambda = \|\mathbf{b}^*\|_2^2$. Let a bar over any vector \mathbf{v} denote the average of the components of \mathbf{v} , so $\bar{\mathbf{v}} = \sum_j v_j$. Note that $\hat{\alpha} = \overline{\mathbf{Y} - \mathbf{S}\hat{\mathbf{b}}}$, and define $\hat{a}^* = \overline{\mathbf{Y} - \mathbf{S}\mathbf{b}^*}$. By our choice of λ , we have that

$$\|\mathbf{Y} - \hat{\alpha}\mathbf{1} - \mathbf{S}\hat{\mathbf{b}}\|_2^2 \leq \|\mathbf{Y} - \hat{a}^*\mathbf{1} - \mathbf{S}\mathbf{b}^*\|_2^2.$$

Noting that for any $\mathbf{v}, \mathbf{u} \in \mathbb{R}^n$, $\mathbf{v}^T(\mathbf{u} - \bar{\mathbf{u}}\mathbf{1}) = (\mathbf{v} - \bar{\mathbf{v}}\mathbf{1})^T\mathbf{u}$, rearranging the inequality above we get

$$\|\alpha^*\mathbf{1} + \mathbf{f}^* - \hat{\alpha}\mathbf{1} - \mathbf{S}\hat{\mathbf{b}}\|_2^2 \leq 2(\varepsilon - \bar{\varepsilon}\mathbf{1})^T\mathbf{S}(\hat{\mathbf{b}} - \mathbf{b}^*) + \|\alpha^*\mathbf{1} + \mathbf{f}^* - \hat{a}^*\mathbf{1} - \mathbf{S}\mathbf{b}^*\|_2^2. \quad (8.21)$$

Now observe that

$$\begin{aligned} \|\alpha^*\mathbf{1} + \mathbf{f}^* - \hat{a}^*\mathbf{1} - \mathbf{S}\mathbf{b}^*\|_2^2 &= \|\mathbf{f}^* - \bar{\mathbf{f}}^*\mathbf{1} - (\mathbf{S}\mathbf{b}^* - \overline{\mathbf{S}\mathbf{b}^*}\mathbf{1})\|_2^2 + n\bar{\varepsilon}^2 \\ &\leq \|\mathbf{f}^* - \mathbf{S}\mathbf{b}^*\|_2^2 + n\bar{\varepsilon}^2. \end{aligned} \quad (8.22)$$

As \mathbf{b}^* is independent of ε , taking expectations of (8.21) yields

$$\text{MSPE}(\hat{\mathbf{b}}) = \frac{2}{n}\mathbb{E}\{(\varepsilon - \bar{\varepsilon}\mathbf{1})^T\mathbf{S}\hat{\mathbf{b}}\} + \frac{1}{n}\mathbb{E}(\|\mathbf{f}^* - \mathbf{S}\mathbf{b}^*\|_2^2) + \frac{\sigma^2}{n}. \quad (8.23)$$

Now using the fact that $\|\hat{\mathbf{b}}\|_2 \leq \|\mathbf{b}^*\|_2$ and applying the Cauchy–Schwarz inequality we have

$$\mathbb{E}_{\varepsilon, \pi, \Psi}\{(\varepsilon - \bar{\varepsilon}\mathbf{1})^T\mathbf{S}\hat{\mathbf{b}}\} \leq \sqrt{\mathbb{E}_{\varepsilon, \pi, \Psi}\{\|\mathbf{S}^T(\varepsilon - \bar{\varepsilon}\mathbf{1})\|_2^2\}}\sqrt{\mathbb{E}(\|\mathbf{b}^*\|_2^2)}.$$

But

$$\begin{aligned} \mathbb{E}_{\varepsilon}(\|\mathbf{S}^T(\varepsilon - \bar{\varepsilon}\mathbf{1})\|_2^2 | \pi, \Psi) &= \mathbb{E}_{\varepsilon}[\text{Tr}\{(\varepsilon - \bar{\varepsilon}\mathbf{1})^T\mathbf{S}\mathbf{S}^T(\varepsilon - \bar{\varepsilon}\mathbf{1})\} | \pi, \Psi] \\ &= \mathbb{E}_{\varepsilon}[\text{Tr}\{(\varepsilon - \bar{\varepsilon}\mathbf{1})(\varepsilon - \bar{\varepsilon}\mathbf{1})^T\mathbf{S}\mathbf{S}^T\} | \pi, \Psi] \\ &= \text{Tr}[\mathbb{E}_{\varepsilon}\{(\varepsilon - \bar{\varepsilon}\mathbf{1})(\varepsilon - \bar{\varepsilon}\mathbf{1})^T\}\mathbf{S}\mathbf{S}^T] \\ &= \sigma^2\|(\mathbf{I} - n^{-1}\mathbf{1}\mathbf{1}^T)\mathbf{S}\|_F^2 \leq \sigma^2\|\mathbf{S}\|_F^2 \leq \sigma^2 nL, \end{aligned}$$

whence

$$\mathbb{E}_{\varepsilon, \pi, \Psi}\{(\varepsilon - \bar{\varepsilon}\mathbf{1})^T\mathbf{S}\hat{\mathbf{b}}\} \leq \sigma\sqrt{c_2 n}. \quad (8.24)$$

Substituting in to (8.23) then gives the result. \square

8.2.2 Logistic regression

We give an analogous result to Theorem 4 for classification problems under logistic loss. Let $\mathbf{X} \in [-1, 1]^{n \times p}$ be the design matrix of predictor variables and let $\mathbf{Y} \in \{0, 1\}^n$ be an associated vector of class labels. We assume the model

$$Y_i \sim \text{Bernoulli}(p_i); \quad \log\left(\frac{p_i}{1-p_i}\right) = f_i,$$

with the Y_i independent for $1 \leq i \leq n$. Define

$$\hat{\mathbf{b}}_{\lambda} = \arg \min_{\mathbf{b}} \frac{1}{n} \sum_{i=1}^n [-Y_i \mathbf{s}_i^T \mathbf{b} + \log\{1 + \exp(\mathbf{s}_i^T \mathbf{b})\}] \quad \text{such that } \|\mathbf{b}\|_2^2 \leq \lambda.$$

Let $\mathcal{E}(\hat{\mathbf{b}}_\lambda)$ denote the excess risk of $\hat{\mathbf{b}}_\lambda$ under logistic loss, so

$$\mathcal{E}(\hat{\mathbf{b}}_\lambda) = \frac{1}{n} \sum_{i=1}^n \left[-p_i \mathbf{s}_i^T \hat{\mathbf{b}}_\lambda + \log\{1 + \exp(\mathbf{s}_i^T \hat{\mathbf{b}}_\lambda)\} \right] - \frac{1}{n} \sum_{i=1}^n \left[-p_i f_i + \log\{1 + \exp(f_i)\} \right].$$

Theorem 15. *Let $\tilde{p} \in \mathbb{R}$ be given by (4.10). Then we have that there exists λ such that*

$$\mathbb{E}_{\mathbf{Y}, \boldsymbol{\pi}, \boldsymbol{\Psi}} \{\mathcal{E}(\hat{\mathbf{b}}_\lambda)\} \leq \frac{c_1}{4L} + \sqrt{\tilde{p}c_2/n}.$$

Proof. We take $\lambda = \|\mathbf{b}^*\|_2^2$. By the definition of $\hat{\mathbf{b}}$ (dropping the subscript λ), we have

$$\frac{1}{n} \sum_{i=1}^n \left[-Y_i \mathbf{s}_i^T \hat{\mathbf{b}} + \log\{1 + \exp(\mathbf{s}_i^T \hat{\mathbf{b}})\} \right] \leq \frac{1}{n} \sum_{i=1}^n \left[-Y_i \mathbf{s}_i^T \mathbf{b}^* + \log\{1 + \exp(\mathbf{s}_i^T \mathbf{b}^*)\} \right].$$

Using this, analogously to (8.21) we get,

$$\mathcal{E}(\hat{\mathbf{b}}) \leq \frac{1}{n} \sum_{i=1}^n (Y_i - p_i) \{\mathbf{S}(\hat{\mathbf{b}} - \mathbf{b}^*)\}_i + \mathcal{E}(\mathbf{b}^*).$$

Let $\boldsymbol{\varepsilon} := \mathbf{Y} - \mathbf{p}$ be the residual vector. Since \mathbf{b}^* is independent of $\boldsymbol{\varepsilon}$, after taking expectations we arrive at

$$\mathbb{E}_{\boldsymbol{\varepsilon}, \boldsymbol{\pi}, \boldsymbol{\Psi}} \{\mathcal{E}(\hat{\mathbf{b}})\} \leq \frac{1}{n} \mathbb{E}_{\boldsymbol{\varepsilon}, \boldsymbol{\pi}, \boldsymbol{\Psi}} (\boldsymbol{\varepsilon}^T \mathbf{S} \hat{\mathbf{b}}) + \mathbb{E}_{\boldsymbol{\pi}, \boldsymbol{\Psi}} \{\mathcal{E}(\mathbf{b}^*)\}.$$

Write $h(a) = \log(1 + e^a)$. By the mean value theorem, we have

$$\begin{aligned} |\mathcal{E}(\mathbf{b}^*)| &= \frac{1}{n} \sum_{i=1}^n |h(\mathbf{s}_i^T \mathbf{b}^*) - h(f_i) - (\mathbf{s}_i^T \mathbf{b}^* - f_i) h'(f_i)| \\ &\leq \frac{1}{n} \sup_{a \in \mathbb{R}} h''(a) \|\mathbf{f}^* - \mathbf{S} \mathbf{b}^*\|_2^2 \leq \frac{c_1}{4L}. \end{aligned}$$

The same argument that leads to (8.24) gives

$$\frac{1}{n} \mathbb{E}_{\boldsymbol{\varepsilon}, \boldsymbol{\pi}, \boldsymbol{\Psi}} (\boldsymbol{\varepsilon}^T \mathbf{S} \hat{\mathbf{b}}) \leq \frac{1}{n} \sqrt{\mathbb{E}_{\boldsymbol{\varepsilon}, \boldsymbol{\pi}, \boldsymbol{\Psi}} (\|\mathbf{S}^T \boldsymbol{\varepsilon}\|_2^2)} \sqrt{c_2/L} \leq \sqrt{\tilde{p}c_2/n}.$$

Collecting together the various inequalities, we get the required result. \square

8.3 Technical lemmas

Lemma 16. *Let $(a_i)_{i=1}^\infty$ and $(b_i)_{i=1}^\infty$ be two sequences of non-negative, non-increasing, real numbers such that there is some $i^* \in \mathbb{N}$ for which*

$$\begin{aligned} a_i &\leq b_i \quad \text{for all } i \leq i^*, \\ a_i &\geq b_i \quad \text{for all } i > i^*. \end{aligned}$$

(i) If

$$\sum_{i=1}^{\infty} a_i = \sum_{i=1}^{\infty} b_i < \infty,$$

and $m \geq 1$, then

$$\sum_{i=1}^{\infty} a_i^m \leq \sum_{i=1}^{\infty} b_i^m.$$

(ii) If $(c_i)_{i=1}^{\infty}$ is a sequence of non-negative, non-decreasing real numbers and

$$\sum_{i=1}^{\infty} b_i \leq \sum_{i=1}^{\infty} a_i < \infty, \quad \sum_{i=1}^{\infty} c_i a_i, \quad \sum_{i=1}^{\infty} c_i b_i < \infty,$$

then

$$\sum_{i=1}^{\infty} c_i a_i \geq \sum_{i=1}^{\infty} c_i b_i.$$

Proof. Note that the sequence $(b_i)_{i=1}^{\infty}$ majorises $(a_i)_{i=1}^{\infty}$ (see page 191 of Steele [2004]). Result (i) follows from applying Schur's majorisation inequality (Steele [2004]; page 201) with the convex function $x \mapsto x^m$ on $[0, \infty)$.

For (ii) we argue,

$$\sum_{i=1}^{i^*} c_i (b_i - a_i) \leq c_{i^*} \sum_{i=1}^{i^*} (b_i - a_i) \leq c_{i^*} \sum_{i>i^*} (a_i - b_i) \leq \sum_{i>i^*} c_i (a_i - b_i). \quad \square$$

Lemma 17. Let $q, p \in \mathbb{N}$ with $q \geq 1$, $p \geq \max\{q, 3\}$. We have

$$\sum_{\ell=1}^{p-1} \ell \left(\frac{\binom{p-1-\ell}{q-1}}{\binom{p-1}{q}} \right)^2 \geq \frac{1}{2(2-q/p)^2} \frac{p^2}{(p-1)^2}.$$

Proof. Let the sequences $(a_\ell)_{\ell=1}^{\infty}$ and $(b_\ell)_{\ell=1}^{\infty}$ be defined by

$$a_\ell = \begin{cases} \left(\frac{\binom{p-1-\ell}{q-1}}{\binom{p-1}{q}} \right)^2 & \text{if } 1 \leq \ell \leq p-1 \\ 0 & \text{otherwise,} \end{cases} \quad b_\ell = \begin{cases} \left(\frac{q}{p-1} \right)^2 & \text{if } \ell \leq \left\lfloor \frac{(p-1)^2}{\{2(p-1)-q\}q} \right\rfloor \\ \frac{q}{2(p-1)-q} - \left(\frac{q}{p-1} \right)^2 \left\lfloor \frac{(p-1)^2}{\{2(p-1)-q\}q} \right\rfloor & \text{if } \ell = \left\lfloor \frac{(p-1)^2}{\{2(p-1)-q\}q} \right\rfloor + 1 \\ 0 & \text{otherwise.} \end{cases}$$

Let the sequence $(c_\ell)_{\ell=1}^{\infty}$ be defined by $c_\ell = \ell$. Note the sequences $(a_\ell)_{\ell=1}^{\infty}$, $(b_\ell)_{\ell=1}^{\infty}$ and $(c_\ell)_{\ell=1}^{\infty}$ satisfy the hypotheses of Lemma 16. Thus

$$\sum_{\ell=1}^{p-1} \ell a_\ell \geq \sum_{\ell=1}^{p-1} \ell b_\ell,$$

and

$$\begin{aligned} \sum_{\ell=1}^{p-1} \ell b_\ell &= \frac{1}{2} \left(\frac{q}{p-1} \right)^2 \left(\left\lfloor \frac{(p-1)^2}{\{2(p-1)-q\}q} \right\rfloor + 1 \right) \left\lfloor \frac{(p-1)^2}{\{2(p-1)-q\}q} \right\rfloor \\ &\quad + \left(\frac{q}{p-1} \right)^2 \left(\frac{(p-1)^2}{\{2(p-1)-q\}q} - \left\lfloor \frac{(p-1)^2}{\{2(p-1)-q\}q} \right\rfloor \right) \left(\left\lfloor \frac{(p-1)^2}{\{2(p-1)-q\}q} \right\rfloor + 1 \right). \end{aligned}$$

Letting $x = (p-1)^2 / [\{2(p-1)-q\}q]$, we have

$$\begin{aligned} \sum_{\ell=1}^{p-1} \ell b_\ell &= \frac{1}{2} (\lfloor x \rfloor + 1) \lfloor x \rfloor + (x - \lfloor x \rfloor) (\lfloor x \rfloor + 1) \\ &= \frac{1}{2} x(x+1) - \frac{1}{2} \{ (x - \lfloor x \rfloor) \lfloor x \rfloor + (x - \lfloor x \rfloor)(x+1) \} + (x - \lfloor x \rfloor) (\lfloor x \rfloor + 1). \end{aligned}$$

Since $1 \geq 1/2 + (x - \lfloor x \rfloor)/2$, we see that

$$(x - \lfloor x \rfloor) (\lfloor x \rfloor + 1) \geq \frac{1}{2} (x - \lfloor x \rfloor) (x + 1 + \lfloor x \rfloor),$$

so

$$\begin{aligned} \sum_{\ell=1}^{p-1} \ell b_\ell &\geq \frac{1}{2} x(x+1) \\ &= \frac{1}{2} \left(\frac{(p-1)^2}{\{2(p-1)-q\}q} + 1 \right) \frac{q}{2(p-1)-q} \\ &= \frac{1}{2(p-1)} \frac{p + \{2 - q/(p-1)\}q - 1}{\{2 - q/(p-1)\}^2} \\ &\geq \frac{1}{2(p-1)} \frac{p+q}{\{2 - q/(p-1)\}^2} \\ &\geq \frac{1}{2(2-q/p)^2} \frac{p^2}{(p-1)^2}. \end{aligned} \quad \square$$

Lemma 18. Let $\kappa(\delta) = \delta^{-a}$ where $a \in [0, 1]$. For $\ell \geq 2$,

$$\left| \frac{\kappa^{(\ell)}(1)}{\ell!} \right| \leq a e^a \frac{1}{\ell^{1-a}}.$$

Proof.

$$\begin{aligned} \left| \frac{\kappa^{(\ell)}(1)}{\ell!} \right| &= \frac{a(a+1) \cdots (a+\ell-1)}{1 \cdot 2 \cdots \ell} \\ &= \frac{a}{\ell} \frac{a+1}{1} \frac{a+2}{2} \cdots \frac{a+\ell-1}{\ell-1}. \end{aligned}$$

By Jensen's inequality

$$\begin{aligned} \frac{1}{\ell-1} \left\{ \log \left(\frac{a+1}{1} \right) + \log \left(\frac{a+2}{2} \right) + \cdots + \log \left(\frac{a+\ell-1}{\ell-1} \right) \right\} \\ \leq \log \left(1 + \frac{a\{1 + \log(\ell-1)\}}{\ell-1} \right), \end{aligned}$$

and

$$\left(1 + \frac{a\{1 + \log(\ell - 1)\}}{\ell - 1}\right)^{\ell-1} \leq \exp[a\{1 + \log(\ell - 1)\}].$$

Thus

$$\left|\frac{\kappa^{(\ell)}(1)}{\ell!}\right| \leq ae^a \frac{(\ell - 1)^a}{\ell} \leq ae^a \frac{1}{\ell^{1-a}}.$$

□