Reduced Label Complexity For Tight ℓ_2 Regression

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Abstract

Given data $X \in \mathbf{b}R^{n \times d}$ and labels $\mathbf{y} \in \mathbf{b}R^n$ the goal is find $\mathbf{w} \in \mathbf{b}R^d$ to minimize $\|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$. We give a polynomial algorithm that, oblivious to \mathbf{y} , throws out $n/(d+\sqrt{n})$ data points and is a (1+d/n)-approximation to optimal in expectation. The motivation is tight approximation with reduced label complexity (number of labels revealed). We reduce label complexity by $\Omega(\sqrt{n})$. Open question: Can label complexity be reduced by $\Omega(n)$ with tight (1+d/n)-approximation?

1 Introduction

In an era of big data, upwards of 10 million data points is not rare. However, labels are costly, especially if humans do the labeling. Nevertheless, we want to have and eat our cake. By this we mean to enjoy the statistical benefits of big data while avoiding the need for big labeling.

Let $X \in \mathbb{R}^{n \times d}$ be a data matrix whose rows are the n data points, $X^{T} = [\mathbf{x}_{1}, \mathbf{x}_{2}, \dots, \mathbf{x}_{n}]$ and let $\mathbf{y} \in \mathbb{R}^{n}$ be the corresponding labels, $\mathbf{y}^{T} = [y_{1}, y_{2}, \dots, y_{n}]$. Typically, poly $(d) \ll n \ll e^{d}$. The age-old goal of ℓ_{2} regression is to find $\mathbf{w}_{*} \in \mathbb{R}^{d}$ satisfying

$$\|\mathbf{X}\mathbf{w}_* - \mathbf{y}\|^2 \le \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$$
 for all $\mathbf{w} \in \mathbb{R}^d$. (1)

We study the label complexity of solving (1), the number of labels in \mathbf{y} that must be revealed to approximate \mathbf{w}_* . To define what "approximate \mathbf{w}_* " means, suppose $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)$ are i.i.d. draws from some joint distribution $D(\mathbf{x}, y)$. The expected squared prediction error of \mathbf{w}_* approaches optimal, with a statistical error O(d/n) (Abu-Mostafa et al., 2012, Problem 3.11). Since \mathbf{w}_* is only accurate to within O(d/n), it suffices to approximate \mathbf{w}_* to within that same error. It is also necessary to do so, otherwise the benefit of having big data is lost. This defines the target approximation regime of interest in large-scale machine learning, one of the primary consumers of regression. We seek $(1 + \epsilon)$ -approximations in the regime $\epsilon \leq d/n$. Allowing for randomness, \mathbf{w} approximates \mathbf{w}_* if

$$\mathbb{E}\left[\|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2\right] \le (1 + d/n)\|\mathbf{X}\mathbf{w}_* - \mathbf{y}\|^2. \tag{2}$$

Via Markov's inequality, (2) implies a 1+O(d/n) approximation with constant probability. We give a polynomial approximation algorithm achieving (2) using fewer than n labels, specifically $\Omega(\sqrt{n})$ fewer labels. Before stating our result, let us survey the landscape of tools available, highlighting the need for new tools because existing methods cannot reduce label complexity in the regime $\epsilon \leq d/n$. There are two settings, consistent regression where $X\mathbf{w}_* = \mathbf{y}$ and inconsistent regression.

Notation. The target matrix X is a fixed $n \times d$ real-valued full rank matrix with no zerorows. Typically, we will assume $poly(d) \ll n \ll e^d$ when framing asymptotic runtimes. Uppercase roman (A, B, C, X, \ldots) are matrices. Lowercase bold $(\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{x}, \mathbf{y}, \mathbf{z}, \ldots)$ are vectors. We write $X^T = [\mathbf{x}_1, \ldots, \mathbf{x}_n]$, where \mathbf{x}_i^T is the *i*th row of X (the data points). The standard Euclidean basis is $\mathbf{e}_1, \mathbf{e}_2, \ldots$ (dimension implied from context). I_k is the $k \times k$ identity and [k] is the set $\{1, \ldots, k\}$.

The SVD decomposes X into a product, $X = U\Sigma V^T$. The left-singular matrix $U \in \mathbb{R}^{n \times d}$ is orthogonal, $U^TU = I_d$. The *i*th leverage score is $\ell_i = \|\mathbf{u}_i\|^2$, where \mathbf{u}_i is the *i*th row of U. The diagonal matrix $\Sigma \in \mathbb{R}^{d \times d}_+$ contains the singular values $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_d > 0$. The right-singular matrix $V \in \mathbb{R}^{d \times d}$ is an orthogonal rotation. The SVD can be computed in time $O(nd \min\{n,d\})$.

The Frobenius norm of A is $\|A\|_F^2 = \sum_{ij} A_{ij}^2 = \operatorname{trace}(A^T A) = \operatorname{trace}(AA^T) = \sum_{i \in [d]} \sigma_i^2(A)$. The operator or spectral norm of A is $\|A\|_2 = \max_{\|\mathbf{x}\|=1} \|A\mathbf{x}\| = \sigma_1(A)$. The condition number of X is $\kappa = \|A\|_2 \|A^{-1}\|_2 = \sigma_1/\sigma_d$. The scaled condition number is $\bar{\kappa}^2 = \sum_i (\sigma_1/\sigma_d)^2$.

The pseudo-inverse $X^{\dagger} = (X^{T}X)^{-1}X^{T} = V\Sigma^{-1}U^{T}$ provides a solution to (1), $\mathbf{w}_{*} = X^{\dagger}\mathbf{y}$. The symmetric operator $XX^{\dagger} = UU^{T}$ projects onto the column space of X. For an orthogonal matrix Q, $Q^{\dagger} = Q^{T}$ and $(Q^{T})^{\dagger} = Q$. We use c, c_{1}, c_{2}, \ldots to generically denote absolute constants whose values may change with each instance.

1.1 Consistent (Realizable) ℓ_2 Regression

When $X\mathbf{w}_* = \mathbf{y}$, relative approximation to the optimal in-sample error is undefined. In this setting, we require relative approximation to the optimal weights \mathbf{w}_* . Pre-conditioning the randomized Kaczmarz algorithm in Strohmer and Vershynin (2009) gives label complexity $d \ln(n\kappa^2/d)$ (recall κ is the conditioning of X).

Theorem 1.1. Set $\mathbf{v} = \mathbf{0}$. Independently sample an index $j \in [n]$ using probabilities $p_i = \|\mathbf{u}_i\|^2/d$ for $i \in [n]$. Do this r times and for each sample perform the projective update

$$\mathbf{v} \leftarrow \mathbf{v} - \frac{\mathbf{u}_j(\mathbf{u}_j^{\mathrm{T}}\mathbf{v} - y_j)}{\|\mathbf{u}_i\|^2}.$$
 (3)

Set $\mathbf{w} = V\Sigma^{-1}\mathbf{v}$. Then, for $r \ge d\ln(n\kappa^2/d)$,

$$\mathbb{E}\left[\|\mathbf{w} - \mathbf{w}_*\|^2\right] \le \frac{d}{n} \|\mathbf{w}_*\|^2. \tag{4}$$

The algorithm in Theorem 1.1 requires at most r labels, yielding the advertised label complexity. Direct use of the result in Strohmer and Vershynin (2009) gives a label complexity $\bar{\kappa}^2 \ln(n/d)$, where $\bar{\kappa}$ is the scaled condition number, $d \leq \bar{\kappa}^2 \leq 1 + (d-1)\kappa^2$. Pre-conditioning brings the condition number inside the log, reducing the label complexity from $O(\kappa^2 d \ln(n/d))$ to $O(d \ln(\kappa^2 n/d))$. An open question is whether one can remove dependence on the conditioning all together.

The runtime in Theorem 1.1 is the sum of $O(nd^2)$ preprocessing to get the leverage scores $\|\mathbf{u}_i\|^2$ and the pre-conditioner $V\Sigma^{-1}$, $O(r\log n)$ to sample the r indices and O(rd) for the r projective updates. The $O(nd^2)$ preprocessing can be prohibitive. Using the ideas in Drineas $et\ al.\ (2012)$, one can use approximate fast pre-conditioning with constant factor approximations to the leverage scores to reduce the preprocessing runtime to $O(nd\ln n)$. The label complexity increases by only a constant factor to $cd\ln(n\kappa^2/d)$, but this constant factor can be relevant to practice.

Pre-conditioned SGD with importance sampling for ℓ_p -regression and minimizing strongly convex functions has been investigated in some detail Yang et al. (2016); Needell et al. (2014); Gorbunov et al. (2020). Theorem 1.1 together with its efficient extension using fast approximate pre-conditioning follows by leveraging ideas from Strohmer and Vershynin (2009); Yang et al. (2016); Drineas et al.

(2012). This is not a main contribution of our paper. However, for completeness, we give the full analysis (including identifying the various constants) in Appendix A.2.

1.2 Inconsistent (Unrealizable) ℓ_2 Regression

Label complexity has received much attention, especially in areas such as active learning, Jacobs et al. (2021); MacKay (1992), and experimental design, Pukelsheim (2006); Wang et al. (2017); Allen-Zhu et al. (2017), with theoretical guarantees being rare on account of the adaptive sampling of data, Castro and Nowak (2008). There are three general approaches to label complexity.

- (a) Throw away outliers based on some form of influence weights, Pena and Yohai (1995). While the practical gains can be considerable, as demonstrated in experiments, all the labels are typically used in determining the outliers and theoretical guarantees are lacking. The typical motivation for identifying outliers is to improve the expected out-of-sample performance by "cleaning" the data. This concern is orthogonal to the main goal of this work whose focus is to minimize the in-sample error without using all the in-sample labels.
- (b) Iteratively solve (1) using low iteration count. If each iteration touches at most one point, the label complexity is bounded by the iteration count. Theorem 1.1 uses this approach. The state-of-the art in iteration count and efficiency is fast approximate pre-conditioned CGD Rokhlin and Tygert (2008); Avron et al. (2012). A data set of size $4d^2$ is subsampled to construct the preconditioner, and then $\kappa \ln(n/d)$ iterations suffice to satisfy (2). However, the subsampling uses random projections to form linear combinations of all the data and labels, and each iteration uses all the labels.
 - An alternative is to extend the algorithm in Theorem 1.1 using a fast approximate preconditioned SGD, as in Yang et al. (2016). While the approach is promising, $\Omega(d \log(1/\epsilon)/\epsilon)$ iterations are needed, resulting in too large a label complexity when $\epsilon \leq d/n$.
- (c) Find a rich coreset, a small set of points on which the (possibly reweighted) coresetregression approximates the full data regression. The active learning paradigm MacKay (1992); Cohn et al. (1994); Freund et al. (1997) adds one point at a time adaptively to the working coreset. This adaptive sampling can exponentially reduce label complexity in classification from d/ϵ to $d\log(d/\epsilon)$. However, the settings are very restricted, such as consistent (separable) homogeneous linear models with data uniform on the sphere, Freund et al. (1997); Dasgupta et al. (2005); Balcan et al. (2006, 2007). Even mild deviation from these settings can result in label complexity reverting to d/ϵ Dasgupta (2005). As with outlier ejection, active learning in machine learning is focused on out-of-sample prediction error for a test distribution. Our focus is tight in-sample fit with minimum label complexity. To this end, one fast random projections efficiently construct coresets of size $O(d/\epsilon)$, Sarlos (2006), but these coresets are linear combinations of all the data. The motivation of random-projection coresets is speed, not label complexity. Row-sampling according to leverage score probabilities (Drineas et al., 2008, Theorem 5) uses a pure coreset of size $\Omega(d \log d/\epsilon^2)$ to produce a $(1 + \epsilon)$ -approximator with constant probability. In a sequence of ensuing results using more refined approaches, this sample complexity has been reduced. First one can start with a constant factor approximation using $O(d \log d)$ samples and improve that to a $(1 + \epsilon)$ approximation using an additional d/ϵ samples. This improves the result in Drineas et al. (2008) to $O(d \log d + d/\epsilon)$ Mahoney (2011). The $d \log d$ is unavoidable by a coupon collector argument. However, using a more subtle linear sample sparsification approach, Chen and Price (2019) gets the row-sample complexity down to O(d) for a 2-approximation, which then gives an $O(d+d/\epsilon)$ label complexity for a $(1+\epsilon)$ -approximation in expectation, the current state

of the art. An interesting result in Derezinski and Warmuth (2018) uses volume sampling to obtain an unbiased (d+1)-approximation using d labels, assuming the data in X are in general position (there is no easy way to extend this analysis to sample more than d points). Volume sampling has also been used in matrix reconstruction Deshpande $et\ al.\ (2006)$. The estimator in Derezinski and Warmuth (2018) is unbiased, hence averaging gives a $(1+\epsilon)$ -approximator with $O(d^2/\epsilon)$ labels. Derezinski and Warmuth (2018) emphasize that jointly sampling rows is essential for getting tight approximation, and then go on to give an efficient algorithm for reverse iterative volume sampling, improving on the volume sampling algorithms in Deshpande and Rademacher (2010); Kulesza and Taskar (2012). Note that only coresets constructed oblivious to the labels \mathbf{y} can reduce label complexity, for example Chen and Price (2019); Derezinski and Warmuth (2018).

The prior results don't work in the stringent $\epsilon \leq d/n$ regime, since they imply label complexity n. New tools are needed for this regime. We give a polynomial algorithm to reduce label complexity by $\Omega(\sqrt{n})$. Our algorithm throws away data while maintaining a provable coreset (a combination of approaches (a) and (c) above). The algorithm is based on the following new tools:

- (i) Tight analysis of the regression error obtained by solving the regression problem on an arbitrary coreset obtained after throwing away k points.
- (ii) A probabilistic argument showing that one can always throw away $\Omega(\sqrt{n})$ points while achieving the target approximation error, reducing label complexity by $\Omega(\sqrt{n})$.
- (iii) The probabilistic arguments use a counterintuitive sampling measure for sets of rows. To realize the reduced label complexity implied by (ii), we develop a polynomial rejection sampling algorithm to throw out a set of size $\Omega(\sqrt{n})$ while attaining the bound in (2).

Lower Bounds. Theorems 13 and 14 in Boutsidis *et al.* (2013) give lower bounds on **y**-agnostic coresets with 1 + d/n approximation ratio. Deterministic **y**-agnostic coresets have at least n - d points (label complexity cannot be reduced more than d). Randomized **y**-agnostic coresets yielding 1 + d/n approximation with constant probability have at least n/d points, so label complexity cannot be reduced by more than cn, where $c \sim (d-1)/d$. Since (2) implies approximation with constant probability, the maximum reduction in label complexity one can hope for is cn.

1.3 Our results

Let A be a matrix formed from a k-subset of the rows in X. That is, $A = S^TX$, where S is a row-sampling matrix whose columns are standard basis vectors, $S = [\mathbf{e}_{i_1}, \mathbf{e}_{i_2}, \dots, \mathbf{e}_{i_k}]$. Recall that $X = U\Sigma V^T$ and let $U_A = S^TU$ be the corresponding rows of U. The partial projection matrix P_A plays an important role in our algorithm,

$$P_{A} = A(X^{T}X)^{-1}A^{T} = U_{A}U_{A}^{T},$$
 (5)

where the last expression follows from using the SVD of X, see (11). The influence of the rows A is

$$p_{\mathcal{A}} = \frac{1}{\mathcal{Z}} \frac{(1 - \|\mathbf{P}_{\mathcal{A}}\|_{2})^{2}}{\|\mathbf{P}_{\mathcal{A}}\|_{2}},\tag{6}$$

where $\mathcal{Z} = \sum_{A} (1 - \|P_A\|_2)^2 / \|P_A\|_2$. Note that the influence does not depend on the labels **y**. Our main result is Theorem 3.1, and the algorithm accompanying Theorem 3.1 is simple to state. Jointly sample k rows A to throw out, using the probability distribution over k-subsets of the rows

in X given by the influences p_A in (6). Let X_A^- be the (deficient) data that remains after throwing out the k rows in A, and let y_A^- be the corresponding labels. Perform a simple regression on this reduced (deficient) data to get regression weights w_A^- . Then, Theorem 3.1 states that

$$\mathbb{E}\left[\left\|\mathbf{X}\mathbf{w}_{\mathbf{A}}^{-}-\mathbf{y}\right\|^{2}\right] \leq \left(1 + \frac{dk^{2}}{(n-dk)^{2}}\right)\left\|\mathbf{X}\mathbf{w}_{*}-\mathbf{y}\right\|^{2}.$$
(7)

Note that the algorithm is oblivious to \mathbf{y} and hence serves to reduce the label complexity by k while delivering the approximation in (7). The main tool in our analysis is Lemma 2.1 which gives an exact analysis of the regression obtained from throwing away an arbitrary set of rows A.

When k=1, the algorithm throws out one data point \mathbf{x}_i using sampling probabilities (influences) $p_i \propto (1-\ell_i)^2/\ell_i$. By throwing out (1/n)th of the information, one expects the error to grow correspondingly, by 1/n. A surprise from (7) is that one can throw away one data point and get only an $O(d/n^2)$ error increase. Prior algorithms that explicitly construct coresets can't guarantee such approximations for coreset sizes smaller than n. This already breaks a barrier on what was previously possible. Setting $dk^2/(n-dk)^2=d/n$ proves that one can throw out $k=n/(d+\sqrt{n})\in\Omega(\sqrt{n})$ data points and get approximation ratio 1+d/n. In Section 2 we prove the result for k=1 illustrating all the main ideas, which are then generalized in Section 3.

As it stands, (7) is an existence result, unless one can efficiently sample A according to p_A . The probabilities p_A depend non-trivially on A through the spectral norm of U_A , and there is no obvious way to jointly sample rows using such complicated probabilities. In Section 4 we give an algorithm to sample exactly from the probabilities p_A . The runtime to generate one sample A satisfying (7) is $O(\mu(n + kd \min\{k, d\}))$, where μ is the average inverse leverage score, a measure of coherence,

$$\mu(X) = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{\ell_i}.$$
 (8)

(ℓ_i are the leverage scores, $\ell_i = \|\mathbf{u}_i\|^2$.) For near uniform leverage scores, $\mu \sim n/d$, and the runtime is $O(n^2/d)$. Ideally, the sampling efficiency should not depend on the input.

The sampling algorithm uses two tools. The first is Theorem 4.1 which is a simple way to sample using probabilities p_A that can be written as a sum of some function over the rows of A, for example sampling according to Frobenius norms, $p_A \propto ||A||_F^2$. Our sampling probabilities cannot be written as a sum over rows, which leads to our second idea of carefully bounding the sampling probabilities so that we can use Theorem 4.1 within a rejection sampling framework.

Remainder of the paper. Next, we briefly discuss some open questions and promising directions. We then proceed to the detailed statement of results and proofs.

1.4 Discussion

Our result for the special case k=1 highlights the need for new tools when the approximation regime is stringent. Constructing a coreset from scratch via some form of sparsification won't work. Carefully throwing away data does work. It is instructive to see what our result in (7) implies for a $(1+\epsilon)$ -approximation in the more relaxed setting where ϵ is a (small) constant. Setting $dk^2/(n-dk)^2=\epsilon$ gives $k=n/(d+\sqrt{d/\epsilon})$, so our algorithm throws away O(n/d) data, retaining a coreset proportional to n. This is much worse than the coreset construction algorithms based on sparsification which only need to retain $O(d/\epsilon)$ points. Coreset construction is better for relaxed approximation and data rejection is better for tight approximation. It is not unusual for different regimes to require different techniques. However it is an open question whether data rejection can compete with coreset construction even for relaxed approximation.

Our algorithm throws out $\Omega(\sqrt{n})$ data and provably gets a (1+d/n)-approximation. There are reasons to suspect that one can throw out cn data points and get (1+d/n)-approximation. (i) The lower bound suggests one only needs to retain n/d data points, hence throwing out (d-1)n/d. (ii) If one can repeatedly throw out one point with the k=1 result continuing to hold in a chaining fashion, one can throw out proportional to n data points (see the comments after Theorem 2.2). Unfortunately, the chaining analysis, being adaptive, is difficult.

Lemma 2.1 is an exact leave-A-out result. Our analysis then bounds $(\mathbf{A}\mathbf{w}_* - \mathbf{y}_{\mathbf{A}})^{\mathrm{T}}\mathbf{Q}(\mathbf{A}\mathbf{w}_* - \mathbf{y}_{\mathbf{A}})$ by $\|\mathbf{Q}\|_2 \|\mathbf{A}\mathbf{w}_* - \mathbf{y}_{\mathbf{A}}\|^2$. This is loose because it does not exploit the coordination between the residual $\mathbf{A}\mathbf{w}_* - \mathbf{y}_{\mathbf{A}}$ and Q. In special cases, e.g. d = 1, one can exploit this coordination to throw out cn data points and get (1 + d/n)-approximation, matching the lower bound. Hence, a more subtle analysis could resolve our main open question of whether one can throw out cn points and get (1 + d/n)-approximation. We used a simple regression for inference on the deficient data. A different inference algorithm might produce stronger results, for example a weighted regression as is used in the coreset construction. Or, an all together new approach is needed.

The (oblivious to \mathbf{y}) influence probabilities in (6) identify the "useless" rows, akin to outlier detection. The innovation in our algorithm is that the useless rows are *jointly* sampled. For coreset construction, joint sampling of rows is essential to get the tightest bounds, and the same is likely true for identifying the useless rows. Thus, the probabilities p_A in (6) may be of general interest to machine learning. Can one more efficiently sample according to complex probabilities like p_A ? Or, are there approximations to p_A that can give the same regression accuracy but are easier to sample from? How does the bound change if approximate sampling probabilities are used instead of p_A ?

This work addresses the transductive setting, where one simply wishes to obtain the optimal in-sample weights \mathbf{w}_* , but using fewer labels. In the inductive setting, one is also interested in the expected prediction error on new data (\mathbf{x}, y) drawn from some distribution. It would be interesting to understand how rejection performs in the inductive setting.

2 Reducing Label Complexity By One

Recall that a k-subset of the rows in X is $A = S^TX$, where $S = [\mathbf{e}_{i_1}, \mathbf{e}_{i_2}, \dots, \mathbf{e}_{i_k}]$. Let \mathbf{y}_A be the corresponding y-values for the data in A, $\mathbf{y}_A = S^T\mathbf{y}$. Using the notation in (Abu-Mostafa et al., 2012, Section 4.3), define X_A^- as the deficient dataset with the rows in A removed. Similarly, we have \mathbf{y}_A^- , the corresponding y-values for the deficient data and \mathbf{w}_A^- , the regression weights obtained from the deficient data,

$$\mathbf{w}_{A}^{-} = \underset{\mathbf{w}}{\operatorname{argmin}} \| \mathbf{X}_{A}^{-} \mathbf{w} - \mathbf{y}_{A}^{-} \|^{2}. \tag{9}$$

The partial projection matrix P_A has an important role in our discussion,

$$P_{A} = A(X^{T}X)^{-1}A^{T}.$$
 (10)

Recall the SVD of X, $X = U\Sigma V^{T}$. Let U_{A} be the rows in U corresponding to the rows A. Then,

$$P_{A} = S^{T}X(X^{T}X)^{-1}X^{T}S = S^{T}UU^{T}S = U_{A}U_{A}^{T},$$
 (11)

and hence $\|P_A\|_2 = \|U_AU_A^T\|_2 \le 1$. Assume $\|P_A\|_2 < 1$. This will be without loss of generality because we never need to remove a set of rows A with $\|P_A\|_2 = 1$. Also assume $0 < \|P_A\|_2$ because if $0 = \|P_A\|_2$ for any A, those rows in A are all **0** and can be thrown out. We need the in-sample error for the deficient weights \mathbf{w}_A^{-} on the full data X. This is the content of the next lemma,

Lemma 2.1. Let \mathbf{w}_* be the weights from the full regression, $\mathbf{w}_* = \underset{\mathbf{w}}{\operatorname{argmin}} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$.

$$\|\mathbf{X}\mathbf{w}_{\mathbf{A}}^{\mathsf{T}} - \mathbf{y}\|^{2} = \|\mathbf{X}\mathbf{w}_{*} - \mathbf{y}\|^{2} + (\mathbf{A}\mathbf{w}_{*} - \mathbf{y}_{\mathbf{A}})^{\mathsf{T}} \mathbf{Q} (\mathbf{A}\mathbf{w}_{*} - \mathbf{y}_{\mathbf{A}}), \tag{12}$$

where, assuming $\|P_A\|_2 < 1$, $Q = (I_k - P_A)^{-1} P_A (I_k - P_A)^{-1} = (I_k - P_A)^{-2} - (I_k - P_A)^{-1}$.

Proof. Note that $X_A^T X_A^T = X^T X - A^T A$, and $X_A^T y_A^T = X^T y - A^T y_A$. The deficient weights \mathbf{w}_A^T are

$$\mathbf{w}_{A}^{-} = (X_{A}^{-T}X_{A}^{-})^{-1}X_{A}^{-T}\mathbf{y}_{A}^{-} = (X_{A}^{-T}X_{A}^{-})^{-1}(X^{T}\mathbf{y} - A^{T}\mathbf{y}_{A}).$$
(13)

Using $\mathbf{w}_* = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$ and the Woodbury matrix inversion identity Woodbury (1950),

$$\mathbf{w}_{\mathbf{A}}^{\mathsf{T}} = (\mathbf{X}^{\mathsf{T}}\mathbf{X} - \mathbf{A}^{\mathsf{T}}\mathbf{A})^{-1}(\mathbf{X}^{\mathsf{T}}\mathbf{y} - \mathbf{A}^{\mathsf{T}}\mathbf{y}_{\mathbf{A}}) \tag{14}$$

$$= [(X^{\mathsf{T}}X)^{-1} + (X^{\mathsf{T}}X)^{-1}A^{\mathsf{T}}(I_k - P_A)^{-1}A(X^{\mathsf{T}}X)^{-1}](X^{\mathsf{T}}\mathbf{y} - A^{\mathsf{T}}\mathbf{y}_A)$$
(15)

$$= \mathbf{w}_* + (\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{A}^{\mathrm{T}}(\mathbf{I}_k - \mathbf{P}_{\mathrm{A}})^{-1}\mathbf{A}\mathbf{w}_* - (\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{A}^{\mathrm{T}}(\mathbf{I}_k - \mathbf{P}_{\mathrm{A}})^{-1}\mathbf{y}_{\mathrm{A}}, \tag{16}$$

where the last expression follows by multiplying out the previous expression and using

$$(I_k - P_A)^{-1}P_A = (I_k - P_A)^{-1}(P_A - I + I) = (I_k - P_A)^{-1} - I.$$
(17)

Note, \mathbf{w}_{A}^{-} is well defined since $I_{k} - P_{A}$ is invertible because $\|P_{A}\|_{2} < 1$. Consider $\|X\mathbf{w}_{A}^{-} - \mathbf{y}\|^{2}$,

$$\|X\mathbf{w}_{A}^{\mathsf{T}} - \mathbf{y}\|^{2} = \|X\mathbf{w}_{*} - \mathbf{y} + X(X^{\mathsf{T}}X)^{-1}A^{\mathsf{T}}(I_{k} - P_{A})^{-1}A\mathbf{w}_{*} - X(X^{\mathsf{T}}X)^{-1}A^{\mathsf{T}}(I_{k} - P_{A})^{-1}\mathbf{y}_{A}\|^{2}.$$
(18)

We get the norms-squared of each of the three terms, plus the cross terms. The residual $X\mathbf{w}_* - \mathbf{y}$ is orthogonal to the columns of X, that is $(X\mathbf{w}_* - \mathbf{y})^T X = \mathbf{0}$. Hence, only one of the cross terms is non-zero. After a little algebra, we get four terms,

$$\|\mathbf{X}\mathbf{w}_{A}^{-}\mathbf{y}\|^{2} = \|\mathbf{X}\mathbf{w}_{*} - \mathbf{y}\|^{2} + \mathbf{w}_{*}^{T}\mathbf{A}^{T}(\mathbf{I}_{k} - \mathbf{P}_{A})^{-1}\mathbf{P}_{A}(\mathbf{I}_{k} - \mathbf{P}_{A})^{-1}\mathbf{A}\mathbf{w}_{*} + \mathbf{y}_{A}^{T}(\mathbf{I}_{k} - \mathbf{P}_{A})^{-1}\mathbf{P}_{A}(\mathbf{I}_{k} - \mathbf{P}_{A})^{-1}\mathbf{y}_{A} - 2\mathbf{w}_{*}^{T}\mathbf{A}^{T}(\mathbf{I}_{k} - \mathbf{P}_{A})^{-1}\mathbf{P}_{A}(\mathbf{I}_{k} - \mathbf{P}_{A})^{-1}\mathbf{y}_{A}.$$

$$= \|\mathbf{X}\mathbf{w}_{*} - \mathbf{y}\|^{2} + (\mathbf{A}\mathbf{w}_{*} - \mathbf{y}_{A})^{T}(\mathbf{I}_{k} - \mathbf{P}_{A})^{-1}\mathbf{P}_{A}(\mathbf{I}_{k} - \mathbf{P}_{A})^{-1}(\mathbf{A}\mathbf{w}_{*} - \mathbf{y}_{A}). \quad (20)$$

The alternate form for Q follows by using (17).

A special case of Lemma 2.1 is when k = 1 (one row is removed). The general case uses similar ideas. When A is just one row, $\mathbf{A} = \mathbf{x}_i^{\mathrm{T}}$, and $\mathbf{P}_{\mathbf{A}} = \mathbf{u}_i^{\mathrm{T}} \mathbf{u}_i = \|\mathbf{u}_i\|^2 = \ell_i$, the leverage score for the *i*th row of X (norm-squared of the corresponding row of the left-singular matrix). Lemma 2.1 gives

$$\|\mathbf{X}\mathbf{w}_{i}^{\mathsf{T}} - \mathbf{y}\|^{2} = \|\mathbf{X}\mathbf{w}_{*} - \mathbf{y}\|^{2} + \frac{\ell_{i}}{(1 - \ell_{i})^{2}} \|\mathbf{x}_{i}^{\mathsf{T}}\mathbf{w}_{*} - \mathbf{y}_{i}\|^{2}$$
 (21)

Define the sampling probability

$$p_i = \frac{1}{\mathcal{Z}} \frac{(1 - \ell_i)^2}{\ell_i},\tag{22}$$

where $\mathcal{Z} = \sum_i (1 - \ell_i)^2 / \ell_i$. Sample a row *i* with probability p_i to throw out. Notice that if $\ell_i = 1$ then this row will never be thrown out, consistent with our assumption that $\|P_A\|_2 < 1$.

Theorem 2.2. For any X, pick row i to throw out with probability p_i . Then,

$$\mathbb{E}\left[\|\mathbf{X}\mathbf{w}_{i}^{-}-\mathbf{y}\|^{2}\right] \leq \left(1 + \frac{d}{(n-d)^{2}}\right)\|\mathbf{X}\mathbf{w}_{*}-\mathbf{y}\|^{2}.$$
(23)

Theorem 2.2 implies one can throw out at least one point and get a $(1 + O(d/n^2))$ -approximation. Recall that our target approximation 1 + d/n.

Proof. Using the definition of p_i and $\sum_i \|\mathbf{x}_i^T \mathbf{w}_* - \mathbf{y}\|^2 = \|\mathbf{X} \mathbf{w}_* - \mathbf{y}\|^2$ gives

$$\mathbb{E}\left[\left\|\mathbf{X}\mathbf{w}_{i}^{-}-\mathbf{y}\right\|^{2}\right] = \left(1 + \frac{1}{\mathcal{Z}}\right) \left\|\mathbf{X}\mathbf{w}_{*}-\mathbf{y}\right\|^{2}.$$
(24)

The result follows if $Z \ge (n-d)^2/d$, which we now prove.

$$\mathcal{Z} = \sum_{i=1}^{n} \frac{(1-\ell_i)^2}{\ell_i} = \sum_{i=1}^{n} \frac{1}{\ell_i} - 2 + \ell_i.$$
 (25)

Since $\sum_i \ell_i = \sum_i \|\mathbf{u}_i\|^2 = d$, $\mathcal{Z} = d - 2n + \sum_i 1/\ell_i$. Therefore, we wish to find the minimum possible value of $\sum_i 1/\ell_i$ subject to the constraint $0 < \ell_i \le 1$ and $\sum_i \ell_i = d$. Let us suppose that this minimum is attained at some values $\ell_{1*}, \ldots, \ell_{n*}$ and for some $i, j, \ell_{i*} < \ell_{j*}$. Suppose $\ell_{i*} = \ell - \varepsilon$ and $\ell_{j*} = \ell + \varepsilon$. After some elementary algebra, one finds that replacing both ℓ_{i*} and ℓ_{j*} by ℓ keeps their sum the same but strictly decreases the sum $1/\ell_{i*} + 1/\ell_{j*}$,

$$\frac{1}{\ell - \varepsilon} + \frac{1}{\ell + \varepsilon} > \frac{2}{\ell}.\tag{26}$$

This contradicts $\ell_{1*}, \ldots, \ell_{n*}$ attaining the minimum for \mathcal{Z} which means the minimum possible value for \mathcal{Z} is attained when $\ell_{1*} = \ell_{2*} = \cdots = \ell_{n*} = d/n$. This gives

$$\mathcal{Z} \ge n \times \frac{(1 - d/n)^2}{(d/n)} = \frac{(n - d)^2}{d},\tag{27}$$

concluding the proof.

Comment. Throwing out just one data point looks trivial, but the result is surprising. A data point contains O(1/n) of the information yet throwing one out increases the error by only $O(1/n^2)$. **Comment.** The same qualitative relative error approximation $1 + cd/(n-d)^2$ continues to hold given relative error approximations to ℓ_i and $(1 - \ell_i)$. A fast relative error approximation to ℓ_i is given in Drineas *et al.* (2012). Can one can get a fast relative error approximation to $(1 - \ell_i)$? **Comment.** The algorithm is oblivious to \mathbf{y} as it should be if we are to reduce label complexity. **Comment.** Chaining this approximation factor by throwing out one point at a time gives

$$\left(1 + \frac{d}{(n-d)^2}\right) \left(1 + \frac{d}{(n-d-1)^2}\right) \left(1 + \frac{d}{(n-d-2)^2}\right) \cdots \left(1 + \frac{d}{(n-d-k+1)^2}\right).$$
(28)

Using $1 + x \le e^x$, this product is at most

$$\exp\left(d\sum_{i=0}^{k-1} \frac{1}{(n-d-i)^2}\right). (29)$$

Bounding the sum by an integral gives

$$\sum_{i=0}^{k-1} \frac{1}{(n-d-i)^2} \le \int_0^k dx \, \frac{1}{(n-d-x)^2} = \frac{k}{(n-d)(n-d-k)}.$$
 (30)

Setting k = (n-d)/2 gives an approximation ratio $\exp(d/(n-d)) \approx 1 + d/(n-d)$ after throwing away about half the data. Such a result ought to be possible, but we don't have a proof for any such chaining approach. Our general analysis in the next section only throws out $\Theta(\sqrt{n})$ points.

3 Reducing Label Complexity by $\Omega(\sqrt{n})$.

The goal in this section is to show that one can reduce label complexity by $\Omega(\sqrt{n})$ while attaining the target approximation ratio of 1 + d/n. We prove that such a set of rows A exists and give a polynomial algorithm to find A. The starting point is Lemma 2.1, which implies

$$\|\mathbf{X}\mathbf{w}_{\mathbf{A}}^{-} - \mathbf{y}\|^{2} \le \|\mathbf{X}\mathbf{w}_{*} - \mathbf{y}\|^{2} + \|(\mathbf{I}_{k} - \mathbf{P}_{\mathbf{A}})^{-1}\mathbf{P}_{\mathbf{A}}(\mathbf{I}_{k} - \mathbf{P}_{\mathbf{A}})^{-1}\|_{2}\|\mathbf{A}\mathbf{w}_{*} - \mathbf{y}_{\mathbf{A}}\|^{2}.$$
 (31)

Let $0 \le \lambda < 1$ be an eigenvalue of P_A . Then,

$$\lambda/(1-\lambda)^2 \ge 0 \tag{32}$$

is an eigenvalue of $(I_k - P_A)^{-1}P_A(I_k - P_A)^{-1}$. We see that $(I_k - P_A)^{-1}P_A(I_k - P_A)^{-1}$ is positive, hence $||(I_k - P_A)^{-1}P_A(I_k - P_A)^{-1}||_2$ is given by its top eigenvalue, which is obtained from the top eigenvalue of P_A , which in turn is $||P_A||_2$ since P_A is non-negative. Hence,

$$\|\mathbf{X}\mathbf{w}_{\mathbf{A}}^{\mathsf{T}} - \mathbf{y}\|^{2} \le \|\mathbf{X}\mathbf{w}_{*} - \mathbf{y}\|^{2} + \frac{\|\mathbf{P}_{\mathbf{A}}\|_{2}}{(1 - \|\mathbf{P}_{\mathbf{A}}\|_{2})^{2}} \|\mathbf{A}\mathbf{w}_{*} - \mathbf{y}_{\mathbf{A}}\|^{2}.$$
 (33)

Define a sampling probability for a subset of rows A by

$$p_{\mathcal{A}} = \frac{1}{\mathcal{Z}} \frac{(1 - \|\mathbf{P}_{\mathcal{A}}\|_{2})^{2}}{\|\mathbf{P}_{\mathcal{A}}\|_{2}},\tag{34}$$

where $\mathcal{Z} = \sum_{A} (1 - \|P_A\|_2)^2 / \|P_A\|_2$. Sample the set of k rows A to throw out with probability p_A . Note that we never throw out an A with $\|P_A\|_2 = 1$, consistent with assuming $\|P_A\|_2 < 1$.

Theorem 3.1. For any X, pick k rows A to throw out with probability p_A . Then, for k < n/d,

$$\mathbb{E}\left[\|\mathbf{X}\mathbf{w}_{\mathbf{A}}^{-} - \mathbf{y}\|^{2}\right] \le \left(1 + \frac{dk^{2}}{(n - dk)^{2}}\right) \|\mathbf{X}\mathbf{w}_{*} - \mathbf{y}\|^{2}.$$
(35)

Set $k = n/(d+\sqrt{n})$ in Theorem 3.1 to get a (1+d/n)-approximation. That is, one can reduce label complexity by $n/(d+\sqrt{n}) \in \Omega(\sqrt{n})$ while attaining the target approximation ratio.

Proof. Taking the expectation in (33) using the probabilities in (34) gives

$$\mathbb{E}\left[\left\|\mathbf{X}\mathbf{w}_{\mathbf{A}}^{-}-\mathbf{y}\right\|^{2}\right] \leq \left\|\mathbf{X}\mathbf{w}_{*}-\mathbf{y}\right\|^{2} + \frac{1}{2}\sum_{\mathbf{A}}\left\|\mathbf{A}\mathbf{w}_{*}-\mathbf{y}_{\mathbf{A}}\right\|^{2}.$$
(36)

Let us evaluate the sum over A in (36). Fix $i \in [n]$. The term $(\mathbf{x}_i^{\mathsf{T}}\mathbf{w}_* - y_i)^2$ appears in $\binom{n-1}{k-1}$ of the As. Hence the sum over A contains $\binom{n-1}{k-1}$ copies of $(\mathbf{x}_i^{\mathsf{T}}\mathbf{w}_* - y_i)^2$ for each i. This means

$$\sum_{\mathbf{A}} \|\mathbf{A}\mathbf{w}_* - \mathbf{y}_{\mathbf{A}}\|^2 = {n-1 \choose k-1} \|\mathbf{X}\mathbf{w}_* - \mathbf{y}\|^2$$
 (37)

and we get

$$\mathbb{E}\left[\left\|\mathbf{X}\mathbf{w}_{\mathbf{A}}^{-}-\mathbf{y}\right\|^{2}\right] \leq \left(1 + \frac{\binom{n-1}{k-1}}{\mathcal{Z}}\right) \left\|\mathbf{X}\mathbf{w}_{*}-\mathbf{y}\right\|^{2}.$$
(38)

The remainder of the proof is to upperbound $\binom{n-1}{k-1}/\mathcal{Z}$. We need a lower bound on \mathcal{Z} .

$$\mathcal{Z} = \sum_{A} \frac{(1 - \|P_A\|_2)^2}{\|P_A\|_2} = \sum_{A} \frac{1}{\|P_A\|_2} + \sum_{A} \|P_A\|_2 - 2n.$$
 (39)

As in the proof of Theorem 2.2, fix the sum $\sum_{A} \|P_A\|_2$. Then the sum $\sum_{A} 1/\|P_A\|_2$ is minimized when each term has the same value, i.e., $\|P_A\|_2 = \sum_{A} \|P_A\|_2/\binom{n}{k}$, the average spectral norm of the partial projection matrices (recall that A has k rows). Define \mathcal{Q} as this average spectral norm,

$$Q = \frac{1}{\binom{n}{k}} \sum_{\mathbf{A}} \|\mathbf{P}_{\mathbf{A}}\|_{2}. \tag{40}$$

Then,

$$\mathcal{Z} \ge \binom{n}{k} \frac{(1-\mathcal{Q})^2}{\mathcal{Q}}.\tag{41}$$

Using (41) in (38) gives

$$\mathbb{E}\left[\|\mathbf{X}\mathbf{w}_{\mathbf{A}}^{-}-\mathbf{y}\|^{2}\right] \leq \left(1 + \frac{k}{n} \frac{\mathcal{Q}}{(1-\mathcal{Q})^{2}}\right) \|\mathbf{X}\mathbf{w}_{*}-\mathbf{y}\|^{2}.$$
(42)

We need an upper bound on \mathcal{Q} . Note $\|P_A\|_2 = \|U_AU_A^T\|_2 = \|U_A\|_2^2$. Therefore,

$$\frac{1}{d} \|\mathbf{U}_{\mathbf{A}}\|_{F}^{2} \le \|\mathbf{P}_{\mathbf{A}}\|_{2} \le \|\mathbf{U}_{\mathbf{A}}\|_{F}^{2}. \tag{43}$$

Since $\|\mathbf{U}_{\mathbf{A}}\|_F^2 = \sum_{j \in \mathbf{A}} \|\mathbf{u}_j\|^2$, we have

$$\frac{1}{d\binom{n}{k}} \sum_{A} \sum_{j \in A} \|\mathbf{u}_j\|^2 \le \mathcal{Q} \le \frac{1}{\binom{n}{k}} \sum_{A} \sum_{j \in A} \|\mathbf{u}_j\|^2. \tag{44}$$

Fix $i \in [n]$. The term $\|\mathbf{u}_j\|^2$ appears in $\binom{n-1}{k-1}$ of the As, hence

$$\sum_{A} \sum_{j \in A} \|\mathbf{u}_j\|^2 = \binom{n-1}{k-1} \sum_{i=1}^n \|\mathbf{u}_i\|^2 = \binom{n-1}{k-1} d, \tag{45}$$

where the last step uses $\sum_{i} \|\mathbf{u}_{j}\|^{2} = d$ (orthogonality of U). Using (45) in (44) gives

$$\frac{k}{n} \le \mathcal{Q} \le \frac{dk}{n}.\tag{46}$$

Finally, using the upper bound for Q in (46) in (42) completes the proof.

Comment. Our analysis of Q in the proof is loose by at most a factor of d, which could \sqrt{d} -factor increase in the data thrown out. Indeed, with Q = k/n, $k = n\sqrt{d}/(\sqrt{d} + \sqrt{n})$ gives approximation 1 + d/n. Getting tighter bounds on the average squared spectral norm of k rows of an orthogonal $n \times d$ matrix would have an impact.

Comment. There is a big gap between the $\Omega(\sqrt{n})$ reduction in label complexity offered in Theorem 3.1 compared to the chaining analysis and lower bound which suggests that $\Omega(n)$ is possible. It is an interesting question whether this gap can be closed.

Comment. Our inference algorithm on the reduced data is simple linear regression, the same inference algorithm used on the full data. One direction for improving the result is to couple the inference algorithm to the data thrown out. Specifically reweighting the left-in data and/or using some form of regularization in the fitting.

Comment. The proof is constructive. However getting all sampling probabilities exactly is exponential, taking $O(\binom{n}{k}kd\min\{k,d\})$ time. We discuss a polynomial sampling algorithm next.

4 Polynomial Sampling Algorithm

We wish to exactly sample from the probability distribution (34) efficiently. The probabilities nontrivially depend on $\|U_A\|_2$ and the spectral norm itself is hard to deal with. We give a sampling algorithm based on rejection whose efficiency depends on the small leverage scores (a measure of incoherence) but is otherwise polynomial. This sampling efficiency can be pre-computed.

Sampling a submatrix using probabilities determined by some nontrivial property of the submatrix is generally not easy. One example is volume sampling Deshpande *et al.* (2006), where the probabilities depend on the product of singular values. One setting where it is easy to sample exactly is when the probability of a set of rows is the sum of some function over the rows. Let $U^{T} = [\mathbf{u}_{1}, \ldots, \mathbf{u}_{n}]$ be a matrix with rows \mathbf{u}_{i} . Let $f(\mathbf{u})$ be a nonnegative function and define the sampling probability for a set of k rows A as proportional to the sum of f over the rows in A,

$$p_{\mathcal{A}} = \frac{1}{\mathcal{Z}} \sum_{i \in \mathcal{A}} f(\mathbf{u}_i), \tag{47}$$

where

$$\mathcal{Z} = \sum_{A} \sum_{i \in A} f(\mathbf{u}_i) = {n-1 \choose k-1} \sum_{i=1}^{n} f(\mathbf{u}_i).$$
 (48)

For any f, one can sample exactly using probabilities p_A in O(n) time.

Theorem 4.1. Sample one row \mathbf{u}_i according to the probabilities

$$p_i = \frac{f(\mathbf{u}_i)}{\sum_{i=1}^n f(\mathbf{u}_i)}.$$
 (49)

Sample k-1 rows (without replacement) uniformly from the $\binom{n-1}{k-1}$ possible (k-1)-subsets of the remaining n-1 rows in U_i^- . For any f, the probability to sample A is given by p_A in (47).

Proof. Consider the set of rows $A^T = [\mathbf{u}_1, \dots, \mathbf{u}_k]$. The same argument applies to any other k rows. We compute the probability to sample A. Conditioning on the first row sampled,

$$\mathbb{P}[A] = \sum_{i=1}^{k} \mathbb{P}[\mathbf{u}_i \text{ is the first row sampled}] \mathbb{P}[A_i^- \text{ are the remaining rows sampled} \mid \mathbf{u}_i]$$
 (50)

$$= \sum_{i=1}^{k} p_i \times \frac{1}{\binom{n-1}{k-1}} \tag{51}$$

$$= \frac{1}{\binom{n-1}{k-1} \sum_{i=1}^{n} f(\mathbf{u}_i)} \sum_{i=1}^{k} f(\mathbf{u}_i)$$
 (52)

$$= p_{A}, (53)$$

where the last step follows from the definitions of p_A and Z.

Comment. Sampling using Frobenius norm probabilities, $p_A \propto \sum_{i \in A} \|\mathbf{u}_i\|^2$ fits the assumptions of the theorem with $f(\mathbf{u}) = \|\mathbf{u}\|^2$. Sampling using inverse sum of leverage scores also fits, where $f(\mathbf{u}) = 1/\|\mathbf{u}\|^2$ in which case $p_A \propto \sum_{i \in A} 1/\|\mathbf{u}_i\|^2$.

We use rejection to sample A according to the probabilities in (34). Here is the algorithm.

- 1: Sampling A using probabilities p_A in (34).
- 2: repeat
- 3: Sample A using Theorem 4.1 and the probabilities q_A given by $f(\mathbf{u}) = 1/\|\mathbf{u}\|^2$,

$$q_{\mathcal{A}} = \frac{1}{\binom{n-1}{k-1} \sum_{j=1}^{n} 1/\|\mathbf{u}_j\|^2} \sum_{i \in \mathcal{A}} 1/\|\mathbf{u}_i\|^2.$$
 (54)

4: Accept A with probability

$$\theta_{A} = \frac{(1 - \|\mathbf{U}_{A}\|_{2}^{2})^{2} / \|\mathbf{U}_{A}\|_{2}^{2}}{\frac{d}{k^{2}} \sum_{i \in A} 1 / \|\mathbf{u}_{i}\|^{2}}.$$
 (55)

5: **until** A is accepted.

First, to show that the rejection sampling is valid, we need that $\theta_{\rm A} \leq 1$. Indeed this is the case. We prove it as follows. Using $\|\mathbf{U}_{\rm A}\|_2^2 \geq \|\mathbf{U}_{\rm A}\|_F^2/d$ and $\|\mathbf{U}_{\rm A}\|_F^2 = \sum_{i \in \mathcal{A}} \|\mathbf{u}_i\|^2$ gives

$$\frac{(1 - \|\mathbf{U}_{\mathbf{A}}\|_{2}^{2})^{2}}{\|\mathbf{U}_{\mathbf{A}}\|_{2}^{2}} \le \frac{(1 - \frac{1}{d}\sum_{i \in \mathbf{A}}\|\mathbf{u}_{i}\|^{2})^{2}}{\frac{1}{d}\sum_{i \in \mathbf{A}}\|\mathbf{u}_{i}\|^{2}} \le \frac{d}{\sum_{i \in \mathbf{A}}\|\mathbf{u}_{i}\|^{2}}.$$
 (56)

We use a convexity argument to bound $d/\sum_{i\in\mathcal{A}} \|\mathbf{u}_i\|^2$,

$$\frac{d}{\sum_{i \in A} \|\mathbf{u}_i\|^2} = \frac{d}{k} \cdot \frac{1}{\frac{1}{k} \sum_{i \in A} \|\mathbf{u}_i\|^2} \le \frac{d}{k} \cdot \frac{1}{k} \sum_{i \in A} 1/\|\mathbf{u}_i\|^2 = \frac{d}{k^2} \sum_{i \in A} 1/\|\mathbf{u}_i\|^2.$$
 (57)

Combining (56) and (57) in (55) establishes that $\theta_A \leq 1$, so the rejection sampling is valid. We now show that the probability distribution of A conditioned on it being accepted is as desired in (34). Indeed,

$$\mathbb{P}[A \mid accept] = \frac{\mathbb{P}[A \cap accept]}{\mathbb{P}[accept]}$$
 (58)

$$= \frac{q_{\rm A}\theta_{\rm A}}{\sum_{\rm A}q_{\rm A}\theta_{\rm A}}.$$
 (59)

For the probability to accept, we have

$$\sum_{A} q_{A} \theta_{A} = \frac{1}{\frac{d}{k^{2}} \binom{n-1}{k-1} \sum_{j=1}^{n} 1/\|\mathbf{u}_{j}\|^{2}} \sum_{A} \frac{(1 - \|\mathbf{U}_{A}\|_{2}^{2})^{2}}{\|\mathbf{U}_{A}\|_{2}^{2}}$$
(60)

$$= \frac{\mathcal{Z}}{\frac{d}{k^2} \binom{n-1}{k-1} \sum_{j=1}^n 1/\|\mathbf{u}_j\|^2}.$$
 (61)

Dividing $q_A \theta_A$ by the above gives

$$\mathbb{P}\left[A \mid accept\right] = \frac{1}{\mathcal{Z}} \frac{(1 - \|U_A\|_2^2)^2}{\|U_A\|_2^2},$$
(62)

as desired. The expected number of trials to accept A is given by $1/\mathbb{P}$ [accept]. The cost of a trial is the time to generate a sample according to the probabilities q_A , which is O(n), plus the time to compute θ_A which is $O(kd \min\{k,d\})$. Hence, the expected runtime is

$$runtime = \frac{O(n + kd \min\{k, d\})}{\mathbb{P}[\text{accept}]}.$$
(63)

We need a lower bound on $\mathbb{P}[\text{accept}]$. For the input matrix X, define a measure of coherence μ ,

$$\mu = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{\|\mathbf{u}_i\|^2},\tag{64}$$

This measure of coherence is the average of the reciprocals of the leverage scores. If the leverage scores are uniform, then $\mu = n/d$. In general, $\mu \ge n/d$ by convexity. The larger μ , the less uniform the leverage scores. The coherence μ captures how many of the leverage scores are small. We get a lower bound for $\mathbb{P}[\text{accept}]$ in terms of μ as follows.

$$\mathbb{P}[\text{accept}] = \frac{k^2}{nd\mu\binom{n-1}{k-1}} \sum_{A} \frac{(1 - \|\mathbf{U}_A\|_2^2)^2}{\|\mathbf{U}_A\|_2^2}$$
 (65)

To get a lower bound for the sum over A, we use $\|U_A\|_2^2 \leq \|U_A\|_F^2$,

$$\sum_{A} \frac{(1 - \|\mathbf{U}_{A}\|_{2}^{2})^{2}}{\|\mathbf{U}_{A}\|_{2}^{2}} \geq \sum_{A} \frac{(1 - \|\mathbf{U}_{A}\|_{F}^{2})^{2}}{\|\mathbf{U}_{A}\|_{F}^{2}}$$

$$= \sum_{A} \|\mathbf{U}_{A}\|_{F}^{2} + \sum_{A} \frac{1}{\|\mathbf{U}_{A}\|_{F}^{2}} - 2\binom{n}{k}$$

$$= \binom{n-1}{k-1}d + \sum_{A} \frac{1}{\|\mathbf{U}_{A}\|_{F}^{2}} - 2\binom{n}{k}$$

$$\geq \binom{n-1}{k-1}d.$$
(66)

where the last step follows from Lemma 4.2 which states that $\sum_{A} 1/\|\mathbf{U}_{A}\|_{F}^{2} > 2\binom{n}{k}$ when $n \geq 8dk$. Since $k \in \Theta(\sqrt{n})$, this means $n \in \Omega(d^{2})$.

$$\mathbb{P}\left[\text{accept}\right] \ge \frac{k^2}{n\mu}.\tag{67}$$

Since $k^2 \in \Theta(n)$, this means that runtime $\in O(\mu(n + kd \min\{k, d\}))$. Since μ is typically of order n/d, the runtime is in $O(n^2/d)$, a polynomial runtime. We now prove the last step in (66).

Lemma 4.2. For
$$n \geq 8dk$$
, $\sum_{\Lambda} \frac{1}{\|\mathbf{U}_{\Lambda}\|_{F}^{2}} - 2\binom{n}{k} \geq 0$.

Proof. Define \mathcal{A}_{bad} as the set of bad As for which $\|\mathbf{U}_{\mathbf{A}}\|_F^2 \geq 1/4$. Then,

$${\binom{n-1}{k-1}}d = \sum_{A} \|U_A\|_F^2 = \sum_{A \in \mathcal{A}_{bad}} \|U_A\|_F^2 + \sum_{A \notin \mathcal{A}_{bad}} \|U_A\|_F^2 \ge \frac{|\mathcal{A}_{bad}|}{4}.$$
 (68)

This means

$$|\mathcal{A}_{\text{bad}}| \le 4d \binom{n-1}{k-1}. \tag{69}$$

We therefore have that

$$\sum_{A} \frac{1}{\|\mathbf{U}_{A}\|_{F}^{2}} = \sum_{A \in \mathcal{A}_{bad}} \frac{1}{\|\mathbf{U}_{A}\|_{F}^{2}} + \sum_{A \notin \mathcal{A}_{bad}} \frac{1}{\|\mathbf{U}_{A}\|_{F}^{2}}$$

$$\geq \sum_{A \notin \mathcal{A}_{bad}} \frac{1}{\|\mathbf{U}_{A}\|_{F}^{2}}$$

$$\geq \left(\binom{n}{k} - |\mathcal{A}_{bad}|\right) \times 4$$

$$\geq 4\binom{n}{k} - 16d\binom{n-1}{k-1}, \tag{70}$$

where the last step uses (69). Subtracting $2\binom{n}{k}$ gives

$$\sum_{A} \frac{1}{\|\mathbf{U}_{A}\|_{F}^{2}} - 2\binom{n}{k} \ge 2\binom{n}{k} - 16d\binom{n-1}{k-1} = 2\binom{n-1}{k-1} \left(\frac{n}{k} - 8d\right). \tag{71}$$

The lemma follows from the assumption $n \geq 8dk$.

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A Consistent ℓ_2 Regression

We prove Theorem 1.1 for consistent regression, including the version with fast preprocessing to get approximate leverage scores and approximate preconditioners. As far as we know Lemma A.2 in the general form stated is new, and may be of independent interest.

A.1 Mathematical Preliminaries

ℓ_2 -Embeddings

The matrix Π is an ϵ -JLT for an orthogonal matrix U if

$$\|\mathbf{I} - \mathbf{U}^{\mathsf{T}} \mathbf{\Pi}^{\mathsf{T}} \mathbf{\Pi} \mathbf{U}\|_{2} \le \epsilon. \tag{72}$$

That is, if IIU is almost orthogonal. The next lemma summarizes some of the consequences of an ϵ -JLT, which are well known, see for example Drineas *et al.* (2010).

Lemma A.1. Let $U \in \mathbb{R}^{n,d}$ be orthogonal and $\Pi \in \mathbb{R}^{n \times r}$. Suppose $\|I - U^T\Pi^T\Pi U\| \le \epsilon < 1$. Then,

- 1. $|1 \sigma_i^2(\Pi \mathbf{U})| \le \epsilon$ and $rank(\Pi \mathbf{U}) = d$.
- 2. Let $\Pi U = \tilde{U} \tilde{\Sigma} \tilde{V}^T$. Then, $\|\tilde{\Sigma} \tilde{\Sigma}^{-1}\| \leq \epsilon/\sqrt{1-\epsilon}$ and $\|I \tilde{\Sigma}^{-2}\| \leq \epsilon/(1-\epsilon)$.
- 3. $\|(\Pi \mathbf{U})^{\dagger} (\Pi \mathbf{U})^{\mathrm{T}}\| \le \epsilon / \sqrt{1 \epsilon}$.
- 4. Let $A = U\Sigma V^T$, where Σ is positive diagonal and V is orthogonal. Then $(\Pi A)^{\dagger} = V\Sigma^{-1}(\Pi U)^{\dagger}$.
- 5. $\|\mathbf{I} (\mathbf{\Pi}\mathbf{U})^{\dagger}(\mathbf{\Pi}\mathbf{U})^{\dagger \mathrm{T}}\| \leq \epsilon/(1-\epsilon)$.

Proof. Part 1 is immediate and implies Part 2 which implies Part 3 because $(\Pi^T U)^{\dagger} = \tilde{V} \tilde{\Sigma}^{-1} \tilde{U}^T$, so

$$\|(\Pi^{\scriptscriptstyle T} U)^\dagger - (\Pi^{\scriptscriptstyle T} U)^{\scriptscriptstyle T}\| = \|\tilde{V} \tilde{\Sigma}^{-1} \tilde{U}^{\scriptscriptstyle T} - \tilde{V} \tilde{\Sigma} \tilde{U}^{\scriptscriptstyle T}\| \leq \|\tilde{\Sigma}^{-1} - \tilde{\Sigma}\|.$$

Part 4 follows from properties of the pseudo-inveerse. For Part 5, using $\Pi^T U = \tilde{U} \tilde{\Sigma} \tilde{V}^T$ and $\tilde{V} \tilde{V}^T = I$ (since $\Pi^T U$ has full rank, so \tilde{V} is a square orthogonal matrix),

$$\|\mathbf{I} - (\mathbf{\Pi}^{\mathsf{T}}\mathbf{U})^{\dagger}(\mathbf{\Pi}^{\mathsf{T}}\mathbf{U})^{\dagger\mathsf{T}}\| = \|\tilde{\mathbf{V}}\tilde{\mathbf{V}}^{\mathsf{T}} - \tilde{\mathbf{V}}\tilde{\boldsymbol{\Sigma}}^{-2}\tilde{\mathbf{V}}^{\mathsf{T}}\| = \|\mathbf{I} - \boldsymbol{\Sigma}^{-2}\| \le \epsilon/(1 - \epsilon),$$

where the last step follows from Part 2.

The next result shows that an ϵ -JLT can be used find a preconditioner.

Lemma A.2. Let $A = U\Sigma V^T$ be $n \times d$, having full rank d. Let $\Pi A = QR$, where Q is any orthogonal matrix and R is invertible. Then $\sigma_i^2(AR^{-1}) = 1/\sigma_{d+1-i}^2(\Pi U)$.

Proof. Consider the SVD of $AR^{-1}R^{-1T}A^{T}$. Using $R^{-1} = (Q^{T}\Pi A)^{-1} = (\Pi A)^{\dagger}Q$,

$$AR^{-1}R^{-1^{\mathrm{T}}}A^{\mathrm{T}} = A(\Pi A)^{\dagger}QQ^{\mathrm{T}}(\Pi A)^{\dagger^{\mathrm{T}}}A^{\mathrm{T}}$$

$$(73)$$

$$= U\Sigma V^{T} V\Sigma^{-1} (\Pi U)^{\dagger} Q Q^{T} (\Pi U)^{\dagger T} \Sigma^{-1} V^{T} V\Sigma U^{T}$$
(74)

$$= U(\Pi U)^{\dagger} Q Q^{T} (\Pi U)^{\dagger^{T}} U^{T}$$

$$(75)$$

$$= U(\Pi U)^{\dagger} (\Pi U)^{\dagger^{\mathrm{T}}} U^{\mathrm{T}}. \tag{76}$$

In the last step QQ^T projects onto the column space of ΠU , hence $QQ^T(\Pi U)^{\dagger T} = (\Pi U)^{\dagger T}$. Using $\Pi U = U_{\Pi U} \Sigma_{\Pi U} V_{\Pi U}^T$, we get $(\Pi U)^{\dagger} (\Pi U)^{\dagger T} = V_{\Pi U} \Sigma_{\Pi U}^{-2} V_{\Pi U}^T$, hence

$$AR^{-1}R^{-1^{T}}A^{T} = UV_{\Pi U}\Sigma_{\Pi U}^{-2}V_{\Pi U}^{T}U^{T}.$$
(77)

Since $UV_{\Pi U}$ is orthogonal, we have constructed the SVD of $AR^{-1}R^{-1T}A^{T}$ and so up to a rotation of the row space, we can write down the SVD of AR^{-1} . For some orthogonal $d \times d$ matrix Z,

$$AR^{-1} = UV_{\Pi U} \Sigma_{\Pi U}^{-1} Z^{T}$$

$$\tag{78}$$

That is, the singular values of AR^{-1} are the inverses of the singular values of ΠU .

A useful corollary of Lemma A.2 was observed in Rokhlin and Tygert (2008), namely that AR⁻¹ and ΠU have the same condition number. Indeed,

$$\kappa(AR^{-1}) = \frac{\sigma_1^2(AR^{-1})}{\sigma_d^2(AR^{-1})} = \frac{1/\sigma_d^2(\Pi U)}{1/\sigma_1^2(\Pi U)} = \frac{\sigma_1^2(\Pi U)}{\sigma_d^2(\Pi U)} = \kappa(\Pi U).$$
 (79)

We make heavy use of ϵ -JLTs which can be constructed and applied efficiently. All constructions use some version of a Johnson-Lindenstrauss Transform. A finite collection of points can be embedded into lower dimension while preserving norms to relative error and inner products to additive error.

Lemma A.3 (JLT, Johnson and Lindenstrauss (1984); Achlioptas (2003)). Let $\Pi \in \mathbb{R}^{d \times r}$ be a matrix of independent random signs scaled by $1/\sqrt{r}$. For n points $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$, let $\mathbf{z}_i = \Pi^T \mathbf{x}_i$. For $0 < \epsilon < 1$ and $\beta > 0$, if

$$r \ge \frac{8+4\beta}{\epsilon^2 - 2\epsilon^3/3} \ln(n+1),\tag{80}$$

then, with probability at least $1 - n^{-\beta}$, for all $i, j \in [1, n]$:

$$(1 - \epsilon) \|\mathbf{x}_i - \mathbf{x}_j\|^2 \le \|\mathbf{z}_i - \mathbf{z}_j\|^2 \le (1 + \epsilon) \|\mathbf{x}_i - \mathbf{x}_j\|^2$$
$$|\mathbf{z}_i^{\mathrm{T}} \mathbf{z}_j - \mathbf{x}_i^{\mathrm{T}} \mathbf{x}_j| \le \epsilon (\|\mathbf{x}_i\|^2 + \|\mathbf{x}_j\|^2).$$

The $\ln(n+1)$ comes from adding **0** to the points which preserves all norms. Also, $\mathbf{x}_i^{\mathrm{T}}\mathbf{x}_j = \frac{1}{2}(\|\mathbf{x}_i\|^2 + \|\mathbf{x}_j\|^2 - \|\mathbf{x}_i - \mathbf{x}_j\|^2)$, hence inner products are preserved to additive error $\epsilon(\|\mathbf{x}_i\|^2 + \|\mathbf{x}_j\|^2)$.

Using this result, we can get ℓ_2 -subspace embeddings using a variety of constructions. The one we will use is an oblivious fast-Hadamard subspace embedding known as the Subsampled Random Hadamard Transform (SRHT). A result from Tropp (2011) which refines earlier results Ailon and Rauhut (2014) is given in next lemma which is an application of Lemmas 3.3 and 3.4 in Tropp (2011). The runtime in the lemma is established in Ailon and Liberty (2013).

Lemma A.4 ((Tropp, 2011, Lemmas 3.3 and 3.4)). Fix $0 < \varepsilon \le \frac{1}{2}$. Let $U \in \mathbb{R}^{n \times d}$ be orthogonal and $\Pi_H \in \mathbb{R}^{r \times n}$ an SRHT with embedding dimension r satisfying:

$$r \ge \frac{12}{5\varepsilon^2} \left(\sqrt{d} + \sqrt{8\ln(3n/\gamma)} \right)^2 \ln d \in O\left(\frac{\ln d}{\varepsilon^2} (d + \ln(n/\gamma)) \right). \tag{81}$$

Then, with probability at least $1 - \gamma$, Π_H is an ϵ -JLT for U,

$$\|\mathbf{I} - \mathbf{U}^{\mathsf{T}} \mathbf{\Pi}_{\mathsf{H}}^{\mathsf{T}} \mathbf{\Pi}_{\mathsf{H}} \mathbf{U}\|_{2} \le \varepsilon. \tag{82}$$

Further, the product $\Pi_H A$ can be computed in time $\textit{O}(\textit{nd} \ln r)$ for any matrix $A \in \mathbb{R}^{n \times d}$.

Note that the SHRT Π_H is constructed obliviously of U. We use the notation ϵ -FJLT for such JLTs that can be applied fast, to distinguish it from the regular ϵ -JLT in Lemma A.3.

A.2 Randomized Pre-Conditioned Kaczmarz

We first consider the consistent case, that is, there exists \mathbf{w}_* for which

$$X\mathbf{w}_* = \mathbf{y}.\tag{83}$$

Equivalently, for any invertible matrix D, we can solve $DX\mathbf{w} = D\mathbf{y}$. The idea is to sample not using row-norms of X, but sample using row-norms of some orthogonal basis for the column-space of X. Let $X = U\Sigma V^{T}$. If we solve \mathbf{v}_{*} satisfying $U\mathbf{v}_{*} = \mathbf{y}$, then we recover \mathbf{w}_{*} using

$$\mathbf{w}_* = \mathbf{V}\Sigma^{-1}\mathbf{v}_*. \tag{84}$$

U is well conditioned so randomized Kaczmarz has a label complexity $d \log(1/\epsilon)$ and runtime $d^2 \log(1/\epsilon)$. The problem is getting U is expensive. However, to identify the rows we need, we don't need U, we just need the leverage scores. And a fast constant factor approximation to the leverage scores will do. This can be accomplished via two JLT's, one for the column-space and one for the row space, Drineas *et al.* (2012).

Let $\Pi_1 \in \mathbb{R}^{r_1 \times n}$ with $r_1 \in O(d \ln d)$ be an ϵ -FJLT for U satisfying

$$\|\mathbf{I} - (\Pi_1 \mathbf{U})^{\mathrm{T}} \Pi_1 \mathbf{U}\| \le \frac{1}{2}.$$
 (85)

The matrix $X_1 = \Pi_1 X$ can be computed in $O(nd \log r_1) = O(nd \log d)$. There are $Q \in \mathbb{R}^{r_1 \times d}$, $T \in \mathbb{R}^{d \times d}$, $P \in \mathbb{R}^{d \times d}$ such that

$$\Pi_1 X = QTP = QR, \tag{86}$$

where Q is orthogonal, T is upper triangular, P is a permutation matrix and R = TP. The reason writing R as the product TP is that one can apply R^{-1} or $(R^{-1})^T$ to any vector \mathbf{x} in $O(d^2)$ without explictly computing R^{-1} . This is because a permutation matrix is orthogonal so $R^{-1} = P^T T^{-1}$ and applying the inverse of an upper triangular $d \times d$ matrix can be done efficiently in $O(d^2)$ Golub and van Loan (1996). Also note,

$$R^{-1} = (Q^{T}\Pi_{1}X)^{-1} = (\Pi_{1}X)^{\dagger}(Q^{T})^{\dagger} = (\Pi_{1}X)^{\dagger}Q.$$
(87)

We now estimate the row-norms of XR⁻¹ to relative error by applying a JLT to the rows. Specifically let $\Pi_2 \in \mathbb{R}^{d \times r_2}$ be a JLT with $r_2 \in O(\log n)$, satisfying

$$\frac{1}{2} \|\mathbf{e}_i^{\mathsf{T}} \mathbf{X} \mathbf{R}^{-1}\|^2 \le \|\mathbf{e}_i^{\mathsf{T}} \mathbf{X} \mathbf{R}^{-1} \mathbf{\Pi}_2\|^2 \le \frac{3}{2} \|\mathbf{e}_i^{\mathsf{T}} \mathbf{X} \mathbf{R}^{-1}\|^2.$$
 (88)

That is, we can estimate all the row-norms in XR⁻¹ to within constant relative error by using the row-norms in XR⁻¹ Π_2 . We can compute XR⁻¹ Π_2 in runtime $O(ndr_2) = O(nd\log n)$. Hence, in $O(nd\log n + d^2\log n)$ we can compute $\hat{\ell}_1, \ldots, \hat{\ell}_n$, where

$$\hat{\ell}_i = \left\| \mathbf{e}_i^{\mathrm{T}} \mathbf{X} \mathbf{R}^{-1} \mathbf{\Pi}_2 \right\|^2. \tag{89}$$

The reason we introduce these quantities $\hat{\ell}_i$ is that they approximate to within relative error the leverage scores of X. Consider $\|\mathbf{e}_i^{\mathrm{T}}\mathbf{X}\mathbf{R}^{-1}\|^2$,

$$\|\mathbf{e}_i^{\mathsf{T}}\mathbf{X}\mathbf{R}^{-1}\|^2 = \|\mathbf{e}_i^{\mathsf{T}}\mathbf{X}(\mathbf{\Pi}_1\mathbf{X})^{\dagger}\mathbf{Q}\|^2$$
(90)

$$= \mathbf{e}_i^{\mathrm{T}} \mathbf{X} (\Pi_1 \mathbf{X})^{\dagger} \mathbf{Q} \mathbf{Q}^{\mathrm{T}} ((\Pi_1 \mathbf{X})^{\dagger})^{\mathrm{T}} \mathbf{X}^{\mathrm{T}} \mathbf{e}_i$$
 (91)

$$= \mathbf{e}_i^{\mathrm{T}} \mathbf{X} (\Pi_1 \mathbf{X})^{\dagger} ((\Pi_1 \mathbf{X})^{\dagger})^{\mathrm{T}} \mathbf{X}^{\mathrm{T}} \mathbf{e}_i$$
 (92)

$$= \|\mathbf{e}_i^{\mathrm{T}} \mathbf{X} (\Pi_1 \mathbf{X})^{\dagger} \|^2. \tag{93}$$

Since $\Pi_1 X = \Pi_1 U \Sigma V^T$,

$$X(\Pi_1 X)^{\dagger} = U \Sigma V^{\mathsf{T}} V \Sigma^{-1} (\Pi_1 U)^{\dagger} = U (\Pi_1 U)^{\dagger}. \tag{94}$$

Therefore,

$$\|\mathbf{e}_i^{\mathrm{T}} \mathbf{X} \mathbf{R}^{-1}\|^2 = \mathbf{e}_i^{\mathrm{T}} \mathbf{U} (\mathbf{\Pi}_1 \mathbf{U})^{\dagger} (\mathbf{\Pi}_1 \mathbf{U})^{\dagger^{\mathrm{T}}} \mathbf{U}^{\mathrm{T}} \mathbf{e}_i$$
(95)

By Part 5 of Lemma A.1, $(\Pi_1 \mathbf{U})^{\dagger}(\Pi_1 \mathbf{U})^{\dagger^{\mathrm{T}}} \approx \mathbf{I}_d$. That means the row norms of $\mathbf{X}\mathbf{R}^{-1}$ are approximately the statistical leverage scores $\|\mathbf{e}_i \mathbf{U}\|^2$. In fact, the estimator in (93) is exactly the one analyzed in Drineas et al. (2012) to obtain an efficient approximation to the leverage scores. This means XR^{-1} is well conditioned.

We can now state the randomized Kaczmarz algorithm. In a nutshell, sample rows of X using probabilities proportional to $\hat{\ell}_i$, as opposed to proportional to $\|\mathbf{x}_i\|^2$, and perform the projective update using the preconditioned row $\mathbf{x}_i \mathbf{R}^{-1}$. By (93), $\hat{\ell}_i \approx \|\mathbf{x}_i \mathbf{R}^{-1}\|^2$. In effect, we are using Kaczmarz to solve the system $XR^{-1}v = y$ but instead of sampling using row-norms, we are sampling using approximate row-norms. Since XR⁻¹ is well conditioned, the algorithm will have exponential convergence independent of the input-conditioning.

- 1: Construct the matrix R as described above using an ϵ -FJLT for $\mathbb{R}^{n\times d}$.
- 2: Compute the leverage scores $\hat{\ell}_i$ as described in (89).
- 3: Compute the cumulative probabilities $F_k = \sum_{i=1}^k \hat{\ell}_i / \sum_{j=1}^n \hat{\ell}_j$.
- 4: Initialize the weights to $\mathbf{v}_0 = \mathbf{0}$.
- 5: **for** t = 1, ..., K **do**
- Independently sample (with replacement) an index $j \in [n]$ using the probabilities $\hat{\ell}_i / \sum_i \hat{\ell}_i$. Let $\mathbf{q} = \mathbf{x}_j^T \mathbf{R}^{-1} = \mathbf{e}_j^T \mathbf{X} \mathbf{R}^{-1}$ and let $s = y_j$. Perform the projective weight update,

$$\mathbf{v}_{t} = \mathbf{v}_{t-1} - \frac{\mathbf{q}(\mathbf{q}^{\mathrm{T}}\mathbf{v}_{t-1} - s)}{\|q\|^{2}}$$

$$(96)$$

8: **return** $\mathbf{w}_K = \mathbf{R}^{-1} \mathbf{v}_K$.

Each step's runtime is as follows.

- 1: $O(nd \log d)$ to compute $\Pi_1 X$ and then $O(d^3 \log d)$ to get R from a QR-factorization.
- 2: $O(nd \log n + d^2 \log n)$ to get $\hat{\ell}_i$.
- 3: O(n) to get all cumulative probabilities
- 4: O(d).
- 5: **for** t = 1, ..., K **do**
- $O(\log n)$ to sample once using binary search, so $O(K \log n)$ in total.
- Applying R^{-1} is $O(d^2)$ and the projective weight update is O(d), so $O(Kd^2)$ in total.
- 8: Applying R^{-1} is $O(d^2)$

Adding all of the above gives $O(nd \log n + d^3 \log d)$ preprocessing time in steps 1-3 and $O(K(\log n +$ (d^2)) for running the Kaczmarz iterations. The label complexity is K.

Note. In step 6, R^{-1} has to be applied to each of $\mathbf{x}_{j_1}, \mathbf{x}_{j_2}, \dots, \mathbf{x}_{j_K}$, which can be pre-sampled ahead of time since the sampling is independent according to fixed probabilities. This requires solving an upper triangular system with multiple right hand sides,

$$R\left[\mathbf{q}_{1}, \mathbf{q}_{2}, \dots, \mathbf{q}_{K}\right] = \left[\mathbf{x}_{j_{1}}, \mathbf{x}_{j_{2}}, \dots, \mathbf{x}_{j_{K}}\right]. \tag{97}$$

A.3 Input-Independent Exponential Convergence of Kaczmarz

We now state and prove the main result for the consistent case where we use the Algorithm described in the previous section. In a nutshell, the convergence is exponential and does not depend on the conditioning of the input matrix X. We make some simplifying assumptions, which in some cases are almost vacuous. Set the failure probability to $\gamma = 1/n$, assume $n \geq 3$ and $\ln n \leq d$. Setting $\epsilon = 1/2$ in (81) and simplifying, an SRHT with $r_1 \geq 48d \ln d$ is an (1/2)-FJLT for any orthogonal $U \in \mathbb{R}^{n \times d}$, with probability at least 1 - 1/n. Similarly, with $\beta = 1, \epsilon = 1/2$ in (80), Lemma A.3 with $r_2 \geq 72 \ln(1+n)$ gives a norm preserving (1/2)-JLT for any n points in \mathbb{R}^d .

Theorem A.5. With probability at least 1 - 2/n (w.r.t. the random choice of Π_1 and Π_2), the Algorithm in the previous section has the following properties.

- 1. The label complexity is K.
- 2. The preprocessing time is in $O(nd \log n)$.
- 3. The time to run the algorithm for a single right hand side \mathbf{y} is in $O(K(\log n + d^2))$.
- 4. The quality of approximation for $\mathbf{w}_t = R^{-1}\mathbf{v}_t$, where $t \in [K]$ is determined by

$$\mathbb{E}\left[\|\mathbf{v}_{t} - \mathbf{v}_{*}\|^{2}\right] \le \left(1 - \frac{1}{9d}\right)^{t} \|\mathbf{v}_{*}\|^{2}.$$
(98)

Where $\mathbf{v}_* = \mathbf{R}\mathbf{w}_*$ and the expectation is over the K random rows used in the projective updates.

Proof. In the weight update (96), use $s = \mathbf{q}^T \mathbf{v}_*$ and subtract \mathbf{v}_* from both sides giving,

$$\mathbf{v}_{t} - \mathbf{v}_{*} = \left(\mathbf{I}_{d} - \frac{\mathbf{q}\mathbf{q}^{\mathrm{T}}}{\|q\|^{2}}\right) (\mathbf{v}_{t-1} - \mathbf{v}_{*})$$

$$(99)$$

Take the norm-squared of both sides and using $(\mathbf{I}_d - \mathbf{q}\mathbf{q}^{\mathrm{T}}/{\|\mathbf{q}\|}^2)^2 = (\mathbf{I}_d - \mathbf{q}\mathbf{q}^{\mathrm{T}}/{\|\mathbf{q}\|}^2)$ gives

$$\|\mathbf{v}_t - \mathbf{v}_*\|^2 = (\mathbf{v}_{t-1} - \mathbf{v}_*)^{\mathrm{T}} \left(\mathbf{I}_d - \frac{\mathbf{q}_i \mathbf{q}_i^{\mathrm{T}}}{\|q_i\|^2} \right) (\mathbf{v}_{t-1} - \mathbf{v}_*)$$

$$(100)$$

$$= \|\mathbf{v}_{t-1} - \mathbf{v}_*\|^2 - (\mathbf{v}_{t-1} - \mathbf{v}_*)^{\mathrm{T}} \frac{\mathbf{q}\mathbf{q}^{\mathrm{T}}}{\|q\|^2} (\mathbf{v}_{t-1} - \mathbf{v}_*)$$
(101)

Taking the expectation of both sides,

$$\mathbb{E}[\|\mathbf{v}_{t} - \mathbf{v}_{*}\|^{2}] = \|\mathbf{v}_{t-1} - \mathbf{v}_{*}\|^{2} - \sum_{i=1}^{n} \frac{\hat{\ell}_{i}}{\sum_{j=1}^{n} \hat{\ell}_{j}} (\mathbf{v}_{t-1} - \mathbf{v}_{*})^{\mathrm{T}} \frac{\mathbf{q}\mathbf{q}^{\mathrm{T}}}{\|q\|^{2}} (\mathbf{v}_{t-1} - \mathbf{v}_{*}).$$
(102)

Using (88) and noting that $\mathbf{q}_i = \mathbf{e}_i^{\mathrm{T}} \mathbf{X} \mathbf{R}^{-1}$, we have that

$$\frac{1}{2}\|\mathbf{q}_i\|^2 \le \hat{\ell}_i \le \frac{3}{2}\|\mathbf{q}_i\|^2. \tag{103}$$

Therefore $\hat{\ell}_i / \sum_j \hat{\ell}_j \ge \frac{1}{2} \|\mathbf{q}_i\|^2 / \frac{3}{2} \sum_j \|\mathbf{q}_j\|^2$. Using (102) and $\sum_j \|\mathbf{q}_j\|^2 = \|\mathbf{X}\mathbf{R}^{-1}\|_F^2$ gives

$$\mathbb{E}[\|\mathbf{v}_{t} - \mathbf{v}_{*}\|^{2}] = \|\mathbf{v}_{t-1} - \mathbf{v}_{*}\|^{2} - \frac{1}{3\|XR^{-1}\|_{F}^{2}}(\mathbf{v}_{t-1} - \mathbf{v}_{*})^{T} \left(\sum_{i=1}^{n} \mathbf{q}_{i} \mathbf{q}_{i}^{T}\right)(\mathbf{v}_{t-1} - \mathbf{v}_{*}) \quad (104)$$

$$\stackrel{(a)}{=} \|\mathbf{v}_{t-1} - \mathbf{v}_*\|^2 - \frac{1}{3\|XR^{-1}\|_E^2} \|XR^{-1}(\mathbf{v}_{t-1} - \mathbf{v}_*)\|^2$$
(105)

$$\leq \left(1 - \frac{\sigma_d^2(XR^{-1})}{3\|XR^{-1}\|_F^2}\right) \|\mathbf{v}_{t-1} - \mathbf{v}_*\|^2.$$
(106)

In (a) we used $\sum_i \mathbf{q}_i \mathbf{q}_i^{\mathrm{T}} = \mathbf{R}^{-1^{\mathrm{T}}} \mathbf{X}^{\mathrm{T}} \mathbf{X} \mathbf{R}^{-1}$. To complete the proof we need to analyze the singular values of $\mathbf{X} \mathbf{R}^{-1}$. By Lemma A.2, $\sigma_i^2(\mathbf{X} \mathbf{R}^{-1}) = 1/\sigma_{d+1-i}^2(\Pi_1 \mathbf{U})$. Since Π_1 is a (1/2)-FJLT for \mathbf{U} , by part 1 in Lemma A.1 $2/3 \le 1/\sigma_i^2(\Pi_1 \mathbf{U}) \le 2$. Hence,

$$\frac{\sigma_d^2(XR^{-1})}{\|XR^{-1}\|_F^2} = \frac{1/\sigma_1^2(\Pi_1 U)}{\sum_{i \in [d]} 1/\sigma_i^2(\Pi_1 U)} \ge \frac{2/3}{\sum_{i \in [d]} 2} = \frac{1}{3d}.$$
 (107)

Using (107) in (106) gives

$$\mathbb{E}\left[\|\mathbf{v}_{t} - \mathbf{v}_{*}\|^{2}\right] \leq \left(1 - \frac{1}{9d}\right) \|\mathbf{v}_{t-1} - \mathbf{v}_{*}\|^{2}.$$
(108)

Since the rows are sampled independently, using iterated expectation gives the final result.

Note that the convergence of \mathbf{v}_t is exponential and input independent, but the condition number does appear in the number of iterations needed to get the error below a threshold. Since $\mathbf{v} = \mathbf{R}\mathbf{w}$,

$$\mathbb{E}\left[\|\mathbf{R}(\mathbf{w}_{t} - \mathbf{w}_{*})\|^{2}\right] \leq \left(1 - \frac{1}{9d}\right)^{t} \|\mathbf{R}\mathbf{w}_{*}\|^{2}.$$
(109)

Since $\sigma_d^2(\mathbf{R}) \|\mathbf{w}\|^2 \le \|\mathbf{R}\mathbf{w}\|^2 \le \sigma_1^2(\mathbf{R}) \|\mathbf{w}\|^2$,

$$\mathbb{E}\left[\|\mathbf{w}_t - \mathbf{w}_*\|^2\right] \le \left(1 - \frac{1}{9d}\right)^t \kappa(\mathbf{R}) \|\mathbf{w}_*\|^2.$$
(110)

Since $\kappa(R) \approx \kappa(X)$ and $\ln(1-1/9d) \approx -1/9d$, setting the right hand side to d/n gives

$$t \approx 9d \ln(n\kappa(X) \|\mathbf{w}_*\|^2 / d). \tag{111}$$

The dependence on κ is now benign, in the logarithm.

Proof of Theorem 1.1

The result in Theorem 1.1 is essentially the same as the one proved in the previous section without the factor of 9. When exact leverage scores are used for sampling and the exact preconditioner R is known (both coming from the exact SVD), then (108) becomes

$$\mathbb{E}\left[\|\mathbf{v}_{t} - \mathbf{v}_{*}\|^{2}\right] \leq \left(1 - \frac{1}{d}\right) \|\mathbf{v}_{t-1} - \mathbf{v}_{*}\|^{2}.$$
 (112)

and (110) becomes

$$\mathbb{E}\left[\|\mathbf{w}_t - \mathbf{w}_*\|^2\right] \le \left(1 - \frac{1}{d}\right)^t \kappa(\mathbf{X}) \|\mathbf{w}_*\|^2.$$
(113)

This then gives Theorem 1.1.