

# Reverse Iterative Volume Sampling for Linear Regression\*

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## Abstract

We study the following basic machine learning task: Given a fixed set of input points in  $\mathbb{R}^d$  for a linear regression problem, we wish to predict a hidden response value for each of the points. We can only afford to attain the responses for a small subset of the points that are then used to construct linear predictions for all points in the dataset. The performance of the predictions is evaluated by the total square loss on all responses (the attained as well as the remaining hidden ones). We show that a good approximate solution to this least squares problem can be obtained from just dimension  $d$  many responses by using a joint sampling technique called volume sampling. Moreover, the least squares solution obtained for the volume sampled subproblem is an unbiased estimator of optimal solution based on all  $n$  responses. This unbiasedness is a desirable property that is not shared by other common subset selection techniques.

Motivated by these basic properties, we develop a theoretical framework for studying volume sampling, resulting in a number of new matrix expectation equalities and statistical guarantees which are of importance not only to least squares regression but also to numerical linear algebra in general. Our methods also lead to a regularized variant of volume sampling, and we propose the first efficient algorithm for volume sampling which makes this technique a practical tool in the machine learning toolbox. Finally, we provide experimental evidence which confirms our theoretical findings.

**Keywords:** volume sampling, linear regression, row sampling, active learning, optimal design

## 1. Introduction

As an introductory case, consider linear regression in one dimension. We are given  $n$  non-zero points  $x_i$ . Each point has a hidden real response (or target value)  $y_i$ . Assume that obtaining the responses is expensive and the learner can afford to request the responses  $y_i$  for only a small number of indices  $i$ . After receiving the requested responses, the learner determines an approximate linear least squares solution. In the one dimensional homogeneous case, this is just a single weight. How many response values does the learner need to request so that the total square loss of its approximate solution on all  $n$  points is “close” to the total loss of the optimal linear least squares solution found with the knowledge of all responses? We will show here that just *one* response suffices if the index  $i$  is chosen proportional to  $x_i^2$ . When the learner uses the approximate solution  $w_i^* = \frac{y_i}{x_i}$ , then its expected loss equals 2 times the loss of the optimum  $w^*$  that is computed based on all responses (See Figure 1). Moreover, the approximate solution  $w_i^*$  is an unbiased estimator for the optimum  $w^*$ :

$$\mathbb{E}_i \left[ \sum_j (x_j \frac{y_i}{x_i} - y_j)^2 \right] = 2 \sum_j (x_j w^* - y_j)^2 \quad \text{and} \quad \mathbb{E}_i \left[ \frac{y_i}{x_i} \right] = w^*, \quad \text{when } P(i) \sim x_i^2.$$

\*. This paper is an expanded version of two conference papers (Dereziński and Warmuth, 2017, 2018).

We will extend these formulas to higher dimensions and to sampling more responses by making use of a joint sampling distribution called *volume sampling*. We next break down our contributions into four parts.

*Least squares with dimension many responses.* Consider the case when the points  $\mathbf{x}_i$  lie in  $\mathbb{R}^d$ . Let  $\mathbf{X}$  denote a full rank  $n \times d$  matrix that has the  $n$  transposed points  $\mathbf{x}_i^\top$  as rows, and let  $\mathbf{y} \in \mathbb{R}^n$  be the vector of responses. Now the goal is to minimize the (total) square loss,

$$L(\mathbf{w}) = \sum_{i=1}^n (\mathbf{x}_i^\top \mathbf{w} - y_i)^2 = \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2,$$

over all linear weight vectors  $\mathbf{w} \in \mathbb{R}^d$ . Let  $\mathbf{w}^*$  denote the optimal such weight vector. We want to minimize the square loss based on a small number of responses we attained for a subset of rows. Again, the learner is initially given the fixed set of  $n$  rows (i.e. fixed design), but none of the responses. It is then allowed to choose a random subset of  $d$  indices,  $S \subseteq \{1..n\}$ , and obtains the responses for the corresponding  $d$  rows. The learner proceeds to find the optimal linear least squares solution  $\mathbf{w}^*(S)$  for the subproblem  $(\mathbf{X}_S, \mathbf{y}_S)$ , where  $\mathbf{X}_S$  is the subset of  $d$  rows of  $\mathbf{X}$  indexed by  $S$  and  $\mathbf{y}_S$  the corresponding  $d$  responses from the response vector  $\mathbf{y}$ . As a generalization of the one-dimensional distribution that chooses an index based on the squared length, set  $S$  of size  $d$  is chosen proportional to the squared volume of the parallelepiped spanned by the rows of  $\mathbf{X}_S$ . This squared volume equals  $\det(\mathbf{X}_S^\top \mathbf{X}_S)$ . Using elementary linear algebra, we will show that *volume sampling* the set  $S$  assures that  $\mathbf{w}^*(S)$  is a good approximation to  $\mathbf{w}^*$  in the following sense: In expectation, the square loss (on all  $n$  row response pairs) of  $\mathbf{w}^*(S)$  is equal  $d + 1$  times the square loss of  $\mathbf{w}^*$  (when  $\mathbf{X}$  is in general position):

$$\mathbb{E}[L(\mathbf{w}^*(S))] = (d + 1) L(\mathbf{w}^*), \quad \text{when } P(S) \sim \det(\mathbf{X}_S^\top \mathbf{X}_S).$$

Furthermore, we will show that for any sampling procedure that attains less than  $d$  responses, the ratio between the expected loss and the loss of the optimum cannot be bounded by a constant.

*Unbiased pseudoinverse estimator.* There is a direct connection between solving linear least squares problems and the pseudoinverse  $\mathbf{X}^+$  of matrix  $\mathbf{X}$ : For an  $n$ -dimensional response vector  $\mathbf{y}$ , the optimal solution is  $\mathbf{w}^* = \operatorname{argmin}_{\mathbf{w}} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 = \mathbf{X}^+ \mathbf{y}$ . Similarly  $\mathbf{w}^*(S) = (\mathbf{X}_S)^+ \mathbf{y}_S$  is the solution for the subproblem  $(\mathbf{X}_S, \mathbf{y}_S)$ . We propose a new implementation of volume sampling called *reverse iterative sampling* which enables a novel proof technique for obtaining elementary expectation formulas for pseudoinverses based on volume sampling.

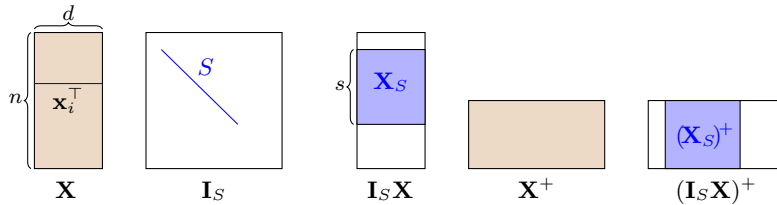


Figure 2: Shapes of the matrices. The indices of  $S$  may not be consecutive.

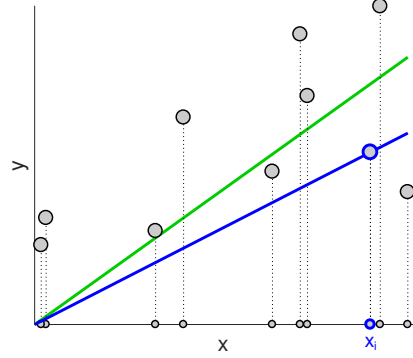


Figure 1: The expected loss of  $w_i^* = \frac{y_i}{x_i}$  (blue line) based on one response  $y_i$  is twice the loss of the optimum  $w^*$  (green line).

Suppose that our goal is to estimate the pseudoinverse  $\mathbf{X}^+$  based on the pseudoinverse of a subset of rows. Recall that for a subset  $S \subseteq \{1..n\}$  of  $s$  row indices (where the size  $s$  is fixed and  $s \geq d$ ), we let  $\mathbf{X}_S$  be the submatrix of the  $s$  rows indexed by  $S$  (see Figure 2). Consider a version of  $\mathbf{X}$  in which all but the rows of  $S$  are zero. This matrix equals  $\mathbf{I}_S \mathbf{X}$ , where the selection matrix  $\mathbf{I}_S$  is an  $n$ -dimensional diagonal matrix with  $(\mathbf{I}_S)_{ii} = 1$  if  $i \in S$  and 0 otherwise.

For the set  $S$  of fixed size  $s \geq d$  row indices chosen proportional to  $\det(\mathbf{X}_S^\top \mathbf{X}_S)$ , we can prove the following two expectation formulas (for the second equality,  $\mathbf{X}$  must be in general position):

$$\mathbb{E}[(\mathbf{I}_S \mathbf{X})^+] = \mathbf{X}^+ \quad \text{and} \quad \mathbb{E} \left[ \underbrace{(\mathbf{X}_S^\top \mathbf{X}_S)^{-1}}_{(\mathbf{I}_S \mathbf{X})^+ (\mathbf{I}_S \mathbf{X})^{+\top}} \right] = \frac{n-d+1}{s-d+1} \underbrace{(\mathbf{X}^\top \mathbf{X})^{-1}}_{\mathbf{X} + \mathbf{X}^{\top}}$$

Note that  $(\mathbf{I}_S \mathbf{X})^+$  has the  $d \times n$  shape of  $\mathbf{X}^+$  where the  $s$  columns indexed by  $S$  contain  $(\mathbf{X}_S)^+$  and the remaining  $n-s$  columns are zero. The expectation of this matrix is  $\mathbf{X}^+$  even though  $(\mathbf{X}_S)^+$  is clearly not a submatrix of  $\mathbf{X}^+$ . This expectation formula now implies that for any size  $s \geq d$ , if  $S$  of size  $s$  is drawn by volume sampling, then  $\mathbf{w}^*(S)$  is an unbiased estimator<sup>1</sup> for  $\mathbf{w}^*$ , i.e.

$$\mathbb{E}[\mathbf{w}^*(S)] = \mathbb{E}[(\mathbf{X}_S)^+ \mathbf{y}_S] = \mathbb{E}[(\mathbf{I}_S \mathbf{X})^+ \mathbf{y}] = \mathbb{E}[(\mathbf{I}_S \mathbf{X})^+] \mathbf{y} = \mathbf{X}^+ \mathbf{y} = \mathbf{w}^*.$$

The second expectation formula can be viewed as a second moment of the pseudoinverse estimator  $(\mathbf{I}_S \mathbf{X})^+$ , and it can be used to compute a useful notion of matrix variance with applications in random matrix theory:

$$\mathbb{E}[(\mathbf{I}_S \mathbf{X})^+ (\mathbf{I}_S \mathbf{X})^{+\top}] - \mathbb{E}[(\mathbf{I}_S \mathbf{X})^+] \mathbb{E}[(\mathbf{I}_S \mathbf{X})^+]^\top = \frac{n-s}{s-d+1} \mathbf{X} + \mathbf{X}^{\top}.$$

*Regularized volume sampling.* We also develop a new regularized variant of volume sampling, which extends reverse iterative sampling to selecting subsets of size smaller than  $d$ , and leads to a useful extension of the above matrix variance formula. Namely, for any  $\lambda \geq 0$ , our  $\lambda$ -regularized procedure for sampling subsets  $S$  of size  $s$  satisfies

$$\mathbb{E}[(\mathbf{X}_S^\top \mathbf{X}_S + \lambda \mathbf{I})^{-1}] \preceq \frac{n-d_\lambda+1}{s-d_\lambda+1} (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1},$$

where  $d_\lambda \stackrel{\text{def}}{=} \text{tr}(\mathbf{X}(\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^\top) \leq d$  is a standard notion of statistical dimension. Crucially, the above bound holds for subset sizes  $s \geq d_\lambda$ , which can be much smaller than the dimension  $d$ .

Under the additional assumption that response vector  $\mathbf{y}$  is generated by a linear transformation distorted with bounded white noise, the expected bound on  $(\mathbf{X}_S^\top \mathbf{X}_S + \lambda \mathbf{I})^{-1}$  leads to strong variance bounds for the ridge regression estimator. Specifically, we prove that when  $\mathbf{y} = \mathbf{X} \tilde{\mathbf{w}} + \boldsymbol{\xi}$ , with  $\boldsymbol{\xi}$  having mean zero and bounded variance  $\text{Var}[\boldsymbol{\xi}] \preceq \sigma^2 \mathbf{I}$ , then if  $S$  is sampled according to  $\lambda$ -regularized volume sampling with  $\lambda \leq \frac{\sigma^2}{\|\tilde{\mathbf{w}}\|^2}$ , we can obtain the following bound on the mean squared prediction error (MSPE):

$$\mathbb{E}_S \mathbb{E}_{\boldsymbol{\xi}} \left[ \frac{1}{n} \|\mathbf{X}(\mathbf{w}_\lambda^*(S) - \tilde{\mathbf{w}})\|^2 \right] \leq \frac{\sigma^2 d_\lambda}{s - d_\lambda + 1},$$

1. For size  $s = d$  volume sampling, the fact that  $\mathbb{E}[\mathbf{w}^*(S)] = \mathbf{w}^*$  can be found in an early paper (Ben-Tal and Teboulle, 1990). They give a direct proof based on Cramer's rule.

where  $\mathbf{w}_\lambda^*(S) = (\mathbf{X}_S^\top \mathbf{X}_S + \lambda \mathbf{I})^{-1} \mathbf{X}_S^\top \mathbf{y}_S$  is the ridge regression estimator for the subproblem  $(\mathbf{X}_S, \mathbf{y}_S)$ . Our new lower bounds show that the above upper bound for regularized volume sampling is essentially optimal with respect to the choice of a subsampling procedure.

*Algorithms and experiments.* The only known polynomial time algorithm for size  $s > d$  volume sampling was recently proposed by Li et al. (2017) with time complexity  $O(n^4 s)$ . In this paper we give two new algorithms using our general framework of reverse iterative sampling: one with deterministic runtime of  $O((n-s+d)nd)$ , and a second one that with high probability finishes in time  $O(nd^2)$ . Thus both algorithms improve on the state-of-the-art by a factor of at least  $n^2$  and make volume sampling nearly as efficient as the comparable i.i.d. sampling technique called leverage score sampling. Our experiments on real datasets confirm the efficiency of our algorithms and show that for small sample sizes  $s$ , volume sampling is more effective than leverage score sampling for the task of subset selection for linear regression.

## 1.1 Related Work

Volume sampling is a type of determinantal point process (DPP) (Kulesza and Taskar, 2012). DPP's have been given a lot of attention in the literature with many applications to machine learning, including recommendation systems (Gartrell et al., 2016) and clustering (Kang, 2013). Many exact and approximate methods for efficiently generating samples from this distribution have been proposed (Deshpande and Rademacher, 2010; Kulesza and Taskar, 2011), making it a useful tool in the design of randomized algorithms. Most of those methods focus on sampling  $s \leq d$  elements. In this paper, we study volume sampling sets of size  $s \geq d$ , which was proposed by Avron and Boutsidis (2013) and motivated with applications in graph theory, linear regression, matrix approximation and more.

The problem of selecting a subset of the rows of the input matrix for solving a linear regression task has been extensively studied in statistics literature under the terms *optimal design* (Fedorov, 1972) and *pool-based active learning* (Sugiyama and Nakajima, 2009). Various criteria for subset selection have been proposed, like A-optimality and D-optimality. For example, A-optimality seeks to minimize  $\text{tr}((\mathbf{X}_S^\top \mathbf{X}_S)^{-1})$ , which is combinatorially hard to optimize exactly. We show that for size  $s \geq d$  volume sampling,  $\mathbb{E}[(\mathbf{X}_S^\top \mathbf{X}_S)^{-1}] = \frac{n-d+1}{s-d+1} (\mathbf{X}^\top \mathbf{X})^{-1}$ , which provides an approximate randomized solution of the sampled inverse covariance matrix rather than just its trace.

In the field of computational geometry a variant of volume sampling was used to obtain optimal bounds for low-rank matrix approximation. In this task, the goal is to select a small subset of rows of a matrix  $\mathbf{X} \in \mathbb{R}^{n \times d}$  (much fewer than the rank of  $\mathbf{X}$ , which is bounded by  $d$ ), so that a good low-rank approximation of  $\mathbf{X}$  can be constructed from those rows. Deshpande et al. (2006) showed that volume sampling of size  $s < d$  index sets obtains optimal multiplicative bounds for this task and polynomial time algorithms for size  $s < d$  volume sampling were given in Deshpande and Rademacher (2010) and Guruswami and Sinop (2012). We show in this paper that for linear regression, fewer than rank many rows do not suffice to obtain multiplicative bounds. This is why we focus on volume sampling sets of size  $s \geq d$  (recall that, for simplicity, we assume that  $\mathbf{X}$  is full rank).

Computing approximate solutions to linear regression has been explored in the domain of numerical linear algebra (see Mahoney (2011) for an overview). Here, multiplicative bounds on the loss of the approximate solution can be achieved via two approaches. The first approach relies on sketching the input matrix  $\mathbf{X}$  and the response vector  $\mathbf{y}$  by multiplying both by the same suitably chosen random matrix. Algorithms which use sketching to generate a smaller input matrix for a given linear regression problem are computationally efficient (Sarlos, 2006; Clarkson and Woodruff,

2013), but they require all of the responses from the original problem to generate the sketch and are thus not suitable for the goal of using as few response values as possible. The second approach is based on subsampling the rows of the input matrix and only asking for the responses of the sampled rows. The learner optimally solves the sampled subproblem<sup>2</sup> and then uses the obtained weight vector for its prediction on all rows. The selected subproblem is known under the term “**b**-agnostic minimal coreset” in (Boutsidis et al., 2013; Drineas et al., 2008) since it is selected without knowing the response vector (denoted as the vector  $\mathbf{b}$ ). The second approach coincides with the goals of this paper but the focus here is different in a number of ways. First, we focus on the smallest sample size for which a multiplicative loss bound is possible: Just  $d$  volume sampled rows are sufficient to achieve a multiplicative bound with a fixed factor, while  $d - 1$  are not sufficient. A second focus here is the efficiency and the combinatorics of volume sampling. The previous work is mostly based on i.i.d. sampling using the statistical leverage scores (Drineas et al., 2012). As we show in this paper, leverage scores are the marginals of volume sampling and any i.i.d. sampling method requires sample size  $\Omega(d \log d)$  to achieve multiplicative loss bounds for linear regression. On the other hand, the rows obtained from volume sampling are *selected jointly* and this makes the chosen subset more informative and brings the required sample size down to  $d$ . Third, we focus on the fact that the estimators produced from volume sampling are unbiased and therefore can be averaged to get more accurate estimators. Using our methods, averaging immediately leads to an unbiased estimator with expected loss  $1 + \epsilon$  times the optimum based on sampling  $d^2/\epsilon$  responses in total. We leave it as an open problem to construct a  $1 + \epsilon$  factor unbiased estimator from sampling only  $O(d/\epsilon)$  responses. If unbiasedness is not a concern, then such an estimator has recently been found (Chen and Price, 2017).

## 1.2 Outline of the Paper

In the next section, we define volume sampling as an instance of a more general procedure we call reverse iterative sampling, and we use this methodology to prove closed form matrix expressions for the expectation of the pseudoinverse estimator  $(\mathbf{I}_S \mathbf{X})^+$  and its square  $(\mathbf{I}_S \mathbf{X})^+ (\mathbf{I}_S \mathbf{X})^{+\top}$ , when  $S$  is sampled by volume sampling. Central to volume sampling is the Cauchy-Binet formula for determinants. As a side, we produce a number of short self-contained proofs for this formula and show that leverage scores are the marginals of volume sampling. Then in Section 3 we formulate the problem of solving linear regression from a small number of responses, and state the upper bound for the expected square loss of the volume sampled least squares estimator (Theorem 8), followed by a discussion and related lower bounds. In Section 3.3, we prove Theorem 8 and an additional related matrix expectation formula. We next discuss in Section 3.4 how unbiased estimators can easily be averaged for improving the expected loss and discuss open problems for constructing unbiased estimators. A new regularized variant of volume sampling is proposed in Section 4, along with the statistical guarantees it offers for computing subsampled ridge regression estimators. Next, we present efficient volume sampling algorithms in Section 5, based on the reverse iterative sampling paradigm, which are then experimentally evaluated in Section 6. Finally, Section 7 concludes the paper by suggesting a future research direction.

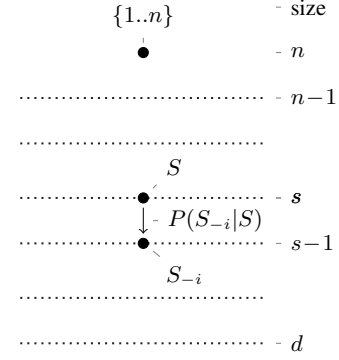
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2. Note that those methods typically require additional rescaling of the subproblem, whereas the techniques proposed in this paper do not require any rescaling.

## 2. Reverse Iterative Sampling

Let  $n$  be an integer dimension. For each subset  $S \subseteq \{1..n\}$  of size  $s$  we are given a matrix formula  $\mathbf{F}(S)$ . Our goal is to sample set  $S$  of size  $s$  using some sampling process and then develop concise expressions for  $\mathbb{E}_{S:|S|=s}[\mathbf{F}(S)]$ . Examples of formula classes  $\mathbf{F}(S)$  will be given below.

We represent the sampling by a directed acyclic graph (DAG), with a single root node corresponding to the full set  $\{1..n\}$ . Starting from the root, we proceed along the edges of the graph, iteratively removing elements from the set  $S$  (see Figure 3). Concretely, consider a DAG with levels  $s = n, n - 1, \dots, d$ . Level  $s$  contains  $\binom{n}{s}$  nodes for sets  $S \subseteq \{1..n\}$  of size  $s$ . Every node  $S$  at level  $s > d$  has  $s$  directed edges to the nodes  $S - \{i\}$  (also denoted  $S_{-i}$ ) at the next lower level. These edges are labeled with a conditional probability vector  $P(S_{-i}|S)$ , where the event  $S$  occurs if the sampling process visits node  $S$  as it traces a (directed) path in the DAG from the root node  $\{1..n\}$  to a node at level  $d$ . Such paths have  $n - d$  edges. It is natural to assign probabilities to shorter paths as well going from any node to a node at a lower level. The probability of such a path is again the product of its edge probabilities. It also follows that the probability  $P(S)$  of visiting node  $S$  (via a path from the root) is the sum of the probabilities of all paths from root to  $S$ . Finally, the probability  $P(\{1..n\})$  of the root node is 1 and more generally, the total probability of all nodes at each layer is 1.



**Figure 3:** Reverse iterative sampling.

We associate a formula  $\mathbf{F}(S)$  with each set node  $S$  in the DAG. The following key equality lets us compute expectations.

**Lemma 1** *If for all  $S \subseteq \{1..n\}$  of size greater than  $d$  we have*

$$\mathbf{F}(S) = \sum_{i \in S} P(S_{-i}|S) \mathbf{F}(S_{-i}),$$

*then for any  $s \in \{d..n\}$ :  $\mathbb{E}_{S:|S|=s}[\mathbf{F}(S)] = \sum_{S:|S|=s} P(S) \mathbf{F}(S) = \mathbf{F}(\{1..n\})$ .*

**Proof** Suffices to show that expectations at successive layers  $s$  and  $s - 1$  are equal for  $s > d$ :

$$\begin{aligned} \sum_{S:|S|=s} P(S) \mathbf{F}(S) &= \sum_{S:|S|=s} P(S) \sum_{i \in S} P(S_{-i}|S) \mathbf{F}(S_{-i}) = \sum_{S:|S|=s} \sum_{i \in S} P(S) P(S_{-i}|S) \mathbf{F}(S_{-i}) \\ &= \sum_{T:|T|=s-1} \underbrace{\sum_{j \notin T} P(T_{+j}) P(T|T_{+j})}_{P(T)} \mathbf{F}(T). \end{aligned}$$

Note that the r.h.s. of the first line has one summand per edge leaving level  $s$ , and the r.h.s. of the second line has one summand per edge arriving at level  $s - 1$ . Now the last equality holds because the edges leaving level  $s$  are exactly those arriving at level  $s - 1$ , and the summand for each edge in both expressions is equivalent.  $\blacksquare$

## 2.1 Volume Sampling

Given a tall full rank matrix  $\mathbf{X} \in \mathbb{R}^{n \times d}$  and a sample size  $s \in \{d..n\}$ , volume sampling chooses subset  $S \subseteq \{1..n\}$  of size  $s$  with probability proportional to squared volume spanned by the columns of submatrix<sup>3</sup>  $\mathbf{X}_S$  and this squared volume equals  $\det(\mathbf{X}_S^\top \mathbf{X}_S)$ . The following theorem uses the above DAG setup to compute the normalization constant for this distribution. Note that all subsets  $S$  of volume 0 will be ignored, since they are unreachable in the proposed sampling procedure.

**Theorem 2** *Let  $\mathbf{X} \in \mathbb{R}^{n \times d}$ , where  $d \leq n$  and  $\det(\mathbf{X}^\top \mathbf{X}) > 0$ . For any set  $S$  of size  $s > d$  for which  $\det(\mathbf{X}_S^\top \mathbf{X}_S) > 0$ , define the probability of the edge from  $S$  to  $S_{-i}$  for  $i \in S$  as:*

$$P(S_{-i}|S) \stackrel{\text{def}}{=} \frac{\det(\mathbf{X}_{S_{-i}}^\top \mathbf{X}_{S_{-i}})}{(s-d) \det(\mathbf{X}_S^\top \mathbf{X}_S)} = \frac{1 - \mathbf{x}_i^\top (\mathbf{X}_S^\top \mathbf{X}_S)^{-1} \mathbf{x}_i}{s-d}, \quad (\text{reverse iterative volume sampling})$$

where  $\mathbf{x}_i^\top$  is the  $i$ -th row of  $\mathbf{X}$ . In this case  $P(S_{-i}|S)$  is a proper probability distribution. If  $\det(\mathbf{X}_S^\top \mathbf{X}_S) = 0$ , then simply set  $P(S_{-i}|S)$  to  $\frac{1}{s}$ . With these definitions,  $\sum_{S:|S|=s} P(S) = 1$  for all  $s \in \{d..n\}$  and the probability of all paths from the root to any subset  $S$  of size at least  $d$  is

$$P(S) = \frac{\det(\mathbf{X}_S^\top \mathbf{X}_S)}{\binom{n-d}{s-d} \det(\mathbf{X}^\top \mathbf{X})}. \quad (\text{volume sampling})$$

The rewrite of the ratio  $\frac{\det(\mathbf{X}_{S_{-i}}^\top \mathbf{X}_{S_{-i}})}{\det(\mathbf{X}_S^\top \mathbf{X}_S)}$  as  $1 - \mathbf{x}_i^\top (\mathbf{X}_S^\top \mathbf{X}_S)^{-1} \mathbf{x}_i$  is Sylvester's Theorem for determinants. Incidentally, this is the only property of determinants used in this section.

The theorem also implies a generalization of the Cauchy-Binet formula to size  $s \geq d$  sets:

$$\sum_{S:|S|=s} \det(\mathbf{X}_S^\top \mathbf{X}_S) = \binom{n-d}{s-d} \det(\mathbf{X}^\top \mathbf{X}). \quad (1)$$

When  $s = d$ , then the binomial coefficient is 1 and the above becomes the vanilla Cauchy-Binet formula. The below proof of the theorem thus results in a minimalist proof of this classical formula as well. The proof uses the reverse iterative sampling (Figure 3) and the fact that all paths from the root to node  $S$  have the same probability. For the sake of completeness we also give a more direct inductive proof of the above generalized Cauchy-Binet formula in Appendix A.

**Proof** First, for any node  $S$  s.t.  $s > d$  and  $\det(\mathbf{X}_S^\top \mathbf{X}_S) > 0$ , the probabilities out of  $S$  sum to 1:

$$\sum_{i \in S} P(S_{-i}|S) = \sum_{i \in S} \frac{1 - \text{tr}((\mathbf{X}_S^\top \mathbf{X}_S)^{-1} \mathbf{x}_i \mathbf{x}_i^\top)}{s-d} = \frac{s - \text{tr}((\mathbf{X}_S^\top \mathbf{X}_S)^{-1} \mathbf{X}_S^\top \mathbf{X}_S)}{s-d} = \frac{s-d}{s-d} = 1.$$

It remains to show the formula for the probability  $P(S)$  of all paths ending at node  $S$ . If  $\det(\mathbf{X}_S^\top \mathbf{X}_S) = 0$ , then one edge on any path from the root to  $S$  has probability 0. This edge goes from a superset of  $S$  with positive volume to a superset of  $S$  that has volume 0. Since all paths have probability 0,  $P(S) = 0$  in this case.

Now assume  $\det(\mathbf{X}_S^\top \mathbf{X}_S) > 0$  and consider any path from the root  $\{1..n\}$  to  $S$ . There are  $(n-s)!$  such paths all going through sets with positive volume. The fractions of determinants in the

3. For sample size  $s = d$ , the rows and columns of  $\mathbf{X}_S$  have the same length and  $\det(\mathbf{X}_S^\top \mathbf{X}_S)$  is also the squared volume spanned by the rows  $\mathbf{X}_S$ .

probabilities along each path telescope and the additional factors accumulate to the same product. So the probability of all paths from the root to  $S$  is the same and the total probability into  $S$  is

$$\frac{(n-s)!}{(n-d)\dots(s-d+1)} \frac{\det(\mathbf{X}_S^\top \mathbf{X}_S)}{\det(\mathbf{X}^\top \mathbf{X})} = \frac{1}{\binom{n-d}{s-d}} \frac{\det(\mathbf{X}_S^\top \mathbf{X}_S)}{\det(\mathbf{X}^\top \mathbf{X})}. \quad \blacksquare$$

An immediate consequence of the above sampling procedure is the following composition property of volume sampling, which states that this distribution is closed under subsampling. We also give a direct proof to highlight the combinatorics of volume sampling.

**Corollary 3** *For any  $\mathbf{X} \in \mathbb{R}^{n \times d}$  and  $n \geq t > s \geq d$ , the following hierarchical sampling procedure:*

$$\begin{aligned} T &\stackrel{t}{\sim} \mathbf{X} && \text{(size } t \text{ volume sampling from } \mathbf{X}\text{),} \\ S &\stackrel{s}{\sim} \mathbf{X}_T && \text{(size } s \text{ volume sampling from } \mathbf{X}_T\text{)} \end{aligned}$$

*returns a set  $S$  which is distributed according to size  $s$  volume sampling from  $\mathbf{X}$ .*

**Proof** We start with the Law of Total Probability and then use the probability formula for volume sampling from the above theorem. Here  $P(T \cap S)$  means the probability of all paths going through node  $T$  at level  $t$  and ending up at the final node  $S$  at level  $s$ . If  $S \not\subseteq T$ , then  $P(T \cap S) = 0$ .

$$\begin{aligned} P(S) &= \sum_{T: S \subseteq T} \overbrace{P(S|T) P(T)}^{P(T \cap S)} \\ &= \sum_{T: S \subseteq T} \frac{\det(\mathbf{X}_S^\top \mathbf{X}_S)}{\binom{t-d}{s-d} \det(\mathbf{X}_T^\top \mathbf{X}_T)} \frac{\det(\mathbf{X}_T^\top \mathbf{X}_T)}{\binom{n-d}{t-d} \det(\mathbf{X}^\top \mathbf{X})} \\ &= \binom{n-s}{t-s} \frac{\det(\mathbf{X}_S^\top \mathbf{X}_S)}{\binom{t-d}{s-d} \binom{n-d}{t-d} \det(\mathbf{X}^\top \mathbf{X})} = \frac{\det(\mathbf{X}_S^\top \mathbf{X}_S)}{\binom{n-d}{s-d} \det(\mathbf{X}^\top \mathbf{X})}. \end{aligned}$$

Note that for all sets  $T$  containing  $S$ , the probability  $P(T \cap S)$  is the same, and there are  $\binom{n-s}{t-s}$  such sets.  $\blacksquare$

The main competitor of volume sampling is i.i.d. sampling of the rows of  $\mathbf{X}$  w.r.t. the statistical leverage scores. For an input matrix  $\mathbf{X} \in \mathbb{R}^{n \times d}$ , the leverage score of the  $i$ -th row  $\mathbf{x}_i^\top$  of  $\mathbf{X}$  is defined as

$$l_i \stackrel{\text{def}}{=} \mathbf{x}_i^\top (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{x}_i.$$

Recall that this quantity appeared in the definition of conditional probability  $P(S_{-i}|S)$  in Theorem 2, where the leverage score was computed w.r.t. the submatrix  $\mathbf{X}_S$ . In fact, there is a more basic relationship between leverage scores and volume sampling: If set  $S$  is sampled according to size  $s = d$  volume sampling, then the leverage score  $l_i$  of row  $i$  is the marginal probability  $P(i \in S)$  of selecting  $i$ -th row into  $S$ . A general formula for the marginals of size  $s$  volume sampling is given in the following proposition:



**Proposition 4** Let  $\mathbf{X} \in \mathbb{R}^{n \times d}$  be a full rank matrix and  $s \in \{d..n\}$ . If  $S \subseteq \{1..n\}$  is sampled according to size  $s$  volume sampling, then for any  $i \in \{1..n\}$ ,

$$P(i \in S) = \frac{s-d}{n-d} + \frac{n-s}{n-d} \overbrace{\mathbf{x}_i^\top (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{x}_i}^{l_i}.$$

**Proof** Instead of  $P(i \in S)$  we will first compute  $P(i \notin S)$ :

$$\begin{aligned} P(i \notin S) &= \sum_{S: |S|=s, i \notin S} \frac{\det(\mathbf{X}_S^\top \mathbf{X}_S)}{\binom{n-d}{s-d} \det(\mathbf{X}^\top \mathbf{X})} \\ &= \sum_{S: |S|=s, i \notin S} \frac{\sum_{T \subseteq S: |T|=d} \det(\mathbf{X}_T^\top \mathbf{X}_T)}{\binom{n-d}{s-d} \det(\mathbf{X}^\top \mathbf{X})} \\ &= \frac{\binom{n-d-1}{s-d} \overbrace{\sum_{T: |T|=d, i \notin T} \det((\mathbf{X}_{-i})_T^\top (\mathbf{X}_{-i})_T)}^{\det(\mathbf{X}_{-i}^\top \mathbf{X}_{-i})}}{\binom{n-d}{s-d} \det(\mathbf{X}^\top \mathbf{X})} \\ &= \frac{n-s}{n-d} (1 - \mathbf{x}_i^\top (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{x}_i), \end{aligned}$$

where we used Cauchy-Binet twice and the fact that every set  $T : |T| = d, i \notin T$  appears in  $\binom{n-d-1}{s-d}$  sets  $S : |S| = s, i \notin S$ . Now, the marginal probability follows from the fact that  $P(i \in S) = 1 - P(i \notin S)$ .  $\blacksquare$

## 2.2 Expectation Formulas for Volume Sampling

All expectations in the remainder of the paper are w.r.t. volume sampling. We use the short-hand  $\mathbb{E}[\mathbf{F}(S)]$  for expectation with volume sampling where the size of the sampled set is fixed to  $s$ . The expectation formulas for two choices of  $\mathbf{F}(S)$  are proven in Theorems 5 and 6. By Lemma 1 it suffices to show  $\mathbf{F}(S) = \sum_{i \in S} P(S_{-i}|S) \mathbf{F}(S_{-i})$  for volume sampling. We also present a related expectation formula (Theorem 7), which is proven later using different techniques.

Recall that  $\mathbf{X}_S$  is the submatrix of rows indexed by  $S \subseteq \{1..n\}$ . We also use a version of  $\mathbf{X}$  in which all but the rows of  $S$  are zeroed out. This matrix equals  $\mathbf{I}_S \mathbf{X}$  where  $\mathbf{I}_S$  is an  $n$ -dimensional diagonal matrix with  $(\mathbf{I}_S)_{ii} = 1$  if  $i \in S$  and 0 otherwise (see Figure 2).

**Theorem 5** Let  $\mathbf{X} \in \mathbb{R}^{n \times d}$  be a tall full rank matrix (i.e.  $n \geq d$ ). For  $s \in \{d..n\}$ , let  $S \subseteq \{1..n\}$  be a size  $s$  volume sampled set over  $\mathbf{X}$ . Then

$$\mathbb{E}[(\mathbf{I}_S \mathbf{X})^+] = \mathbf{X}^+.$$

For the special case of  $s = d$ , this fact was known in the linear algebra literature (Ben-Tal and Teboulle, 1990; Ben-Israel, 1992). It was shown there using elementary properties of the determinant such as Cramer's rule.<sup>4</sup> The proof methodology developed here based on reverse iterative volume

4. Using the composition property of volume sampling (Corollary 3), the  $s > d$  case of the theorem can be reduced to the  $s = d$  case. However, in this paper we give a different self-contained proof for Theorem 5.

sampling is very different. We believe that this fundamental formula lies at the core of why volume sampling is important in many applications. In this work, we focus on its application to linear regression. However, Avron and Boutsidis (2013) discuss many problems where controlling the pseudoinverse of a submatrix is essential. For those applications, it is important to establish variance bounds for the above expectation and volume sampling once again offers very concrete guarantees. We obtain them by showing the following formula, which can be viewed as a second moment for this estimator.

**Theorem 6** *Let  $\mathbf{X} \in \mathbb{R}^{n \times d}$  be a full rank matrix and  $s \in \{d..n\}$ . If size  $s$  volume sampling over  $\mathbf{X}$  has full support, then*

$$\mathbb{E} \left[ \underbrace{(\mathbf{X}_S^\top \mathbf{X}_S)^{-1}}_{(\mathbf{I}_S \mathbf{X})^+ (\mathbf{I}_S \mathbf{X})^{+\top}} \right] = \frac{n-d+1}{s-d+1} \underbrace{(\mathbf{X}^\top \mathbf{X})^{-1}}_{\mathbf{X}^+ \mathbf{X}^{+\top}}.$$

*In the case when volume sampling does not have full support, then the matrix equality “=” above is replaced by the positive-definite inequality “ $\preceq$ ”.*

The condition that size  $s$  volume sampling over  $\mathbf{X}$  has full support is equivalent to  $\det(\mathbf{X}_S^\top \mathbf{X}_S) > 0$  for all  $S \subseteq \{1..n\}$  of size  $s$ . Note that if size  $s$  volume sampling has full support, then size  $t > s$  also has full support. So full support for the smallest size  $d$  (often phrased as  $\mathbf{X}$  being *in general position*) implies that volume sampling w.r.t. any size  $s \geq d$  has full support.

The above theorem immediately gives an expectation formula for the Frobenius norm  $\|(\mathbf{I}_S \mathbf{X})^+\|_F$  of the estimator:

$$\mathbb{E} [\|(\mathbf{I}_S \mathbf{X})^+\|_F^2] = \mathbb{E}[\text{tr}((\mathbf{I}_S \mathbf{X})^+ (\mathbf{I}_S \mathbf{X})^{+\top})] = \frac{n-d+1}{s-d+1} \|\mathbf{X}^+\|_F^2. \quad (2)$$

This norm formula was shown by Avron and Boutsidis (2013), with numerous applications. Theorem 6 can be viewed as a much stronger pre-trace version of the known norm formula. Also our proof techniques are quite different and much simpler. Note that if size  $s$  volume sampling for  $\mathbf{X}$  does not have full support, then (2) becomes an inequality.

We now mention a second application of the above theorem in the context of linear regression for the case when the response vector  $\mathbf{y}$  is modeled as a noisy linear transformation, i.e.,  $\mathbf{y} = \mathbf{X}\tilde{\mathbf{w}} + \boldsymbol{\xi}$  for some  $\tilde{\mathbf{w}} \in \mathbb{R}^d$  and a random noise vector  $\boldsymbol{\xi} \in \mathbb{R}^n$  (detailed discussion in Section 4). In this case the matrix  $(\mathbf{X}_S^\top \mathbf{X}_S)^{-1}$  can be interpreted as the covariance matrix of least-squares estimator  $\mathbf{w}^*(S)$  (for a fixed set  $S$ ) and Theorem 6 gives an exact formula for the covariance matrix of  $\mathbf{w}^*(S)$  under volume sampling. In Section 4, we give an extended version of this result which provides even stronger guarantees for regularized least-squares estimators under this model (Theorem 16).

Note that except for the above application, all results in this paper hold for arbitrary response vectors  $\mathbf{y}$ . By combining Theorems 5 and 6, we can also obtain a covariance-type formula<sup>5</sup> for the pseudoinverse matrix estimator:

$$\begin{aligned} & \mathbb{E}[(\mathbf{I}_S \mathbf{X})^+ - \mathbb{E}[(\mathbf{I}_S \mathbf{X})^+]] (\mathbf{I}_S \mathbf{X})^+ - \mathbb{E}[(\mathbf{I}_S \mathbf{X})^+] \mathbb{E}[(\mathbf{I}_S \mathbf{X})^+]^\top \\ &= \mathbb{E}[(\mathbf{I}_S \mathbf{X})^+ (\mathbf{I}_S \mathbf{X})^{+\top}] - \mathbb{E}[(\mathbf{I}_S \mathbf{X})^+] \mathbb{E}[(\mathbf{I}_S \mathbf{X})^+]^\top \\ &= \frac{n-d+1}{s-d+1} \mathbf{X}^+ \mathbf{X}^{+\top} - \mathbf{X}^+ \mathbf{X}^{+\top} = \frac{n-s}{s-d+1} \mathbf{X}^+ \mathbf{X}^{+\top}. \end{aligned} \quad (3)$$

5. This notion of “covariance” is used in random matrix theory, i.e. for a random matrix  $\mathbf{M}$ , we analyze  $\mathbb{E}[(\mathbf{M} - \mathbb{E}[\mathbf{M}])(\mathbf{M} - \mathbb{E}[\mathbf{M}])^\top]$ . See for example Tropp (2012).

We now give the background for a third matrix expectation formula for volume sampling. Pseudoinverses can be used to compute the projection matrix onto the span of columns of matrix  $\mathbf{X}$ , which is defined as follows:

$$\mathbf{P}_{\mathbf{X}} \stackrel{\text{def}}{=} \mathbf{X} \overbrace{(\mathbf{X}^{\top} \mathbf{X})^{-1} \mathbf{X}^{\top}}^{\mathbf{X}^+}.$$

Applying Theorem 5 leads us immediately to the following unbiased matrix estimator for the projection matrix:

$$\mathbb{E}[\mathbf{X}(\mathbf{I}_S \mathbf{X})^+] = \mathbf{X} \mathbb{E}[(\mathbf{I}_S \mathbf{X})^+] = \mathbf{X} \mathbf{X}^+ = \mathbf{P}_{\mathbf{X}}.$$

Note that this matrix estimator  $\mathbf{X}(\mathbf{I}_S \mathbf{X})^+$  is closely connected to linear regression: It can be used to transform the response vector  $\mathbf{y}$  into the prediction vector  $\hat{\mathbf{y}}(S)$  of subsampled least squares solution  $\mathbf{w}^*(S)$  as follows:

$$\hat{\mathbf{y}}(S) = \mathbf{X} \underbrace{(\mathbf{I}_S \mathbf{X})^+ \mathbf{y}}_{\mathbf{w}^*(S)}.$$

In this case, volume sampling once again provides a covariance-type matrix expectation formula.

**Theorem 7** *Let  $\mathbf{X} \in \mathbb{R}^{n \times d}$  be a full rank matrix. If matrix  $\mathbf{X}$  is in general position and  $S \subseteq \{1..n\}$  is sampled according to size  $d$  volume sampling, then*

$$\mathbb{E}[\underbrace{(\mathbf{X}(\mathbf{I}_S \mathbf{X})^+)^2}_{(\mathbf{I}_S \mathbf{X})^{+\top} \mathbf{X}^{\top} \mathbf{X} (\mathbf{I}_S \mathbf{X})^+}] - \mathbf{P}_{\mathbf{X}} = d(\mathbf{I} - \mathbf{P}_{\mathbf{X}}).$$

*If  $\mathbf{X}$  is not in general position, then the matrix equality “=” is replaced by the positive-definite inequality “ $\succeq$ ”.*

Note that this third expectation formula is limited to sample size  $s = d$ . It is a direct consequence of Theorem 8 given in the next section which relates the expected loss of a subsampled least squares estimator to the loss of the optimum least squares estimator. Unlike the first two formulas given in theorems 5 and 6, its proof does not rely on the methodology of Lemma 1, i.e., on showing that the expectations at all levels of a certain DAG associated with the sampling process are the same. We defer the proof of this third expectation formula to the end of Section 3.3. No extension of this third formula to sample size  $s > d$  is known.

**Proof of Theorem 5** We apply Lemma 1 with  $\mathbf{F}(S) = (\mathbf{I}_S \mathbf{X})^+$ . It suffices to show  $\mathbf{F}(S) = \sum_{i \in S} P(S_{-i}|S) \mathbf{F}(S_{-i})$  for  $P(S_{-i}|S) = \frac{1 - \mathbf{x}_i^{\top} (\mathbf{X}_S^{\top} \mathbf{X}_S)^{-1} \mathbf{x}_i}{s - d}$ , i.e.:

$$(\mathbf{I}_S \mathbf{X})^+ = \sum_{i \in S} \frac{1 - \mathbf{x}_i^{\top} (\mathbf{X}_S^{\top} \mathbf{X}_S)^{-1} \mathbf{x}_i}{s - d} \underbrace{(\mathbf{I}_{S_{-i}} \mathbf{X})^+}_{(\mathbf{X}_{S_{-i}}^{\top} \mathbf{X}_{S_{-i}})^{-1} (\mathbf{I}_{S_{-i}} \mathbf{X})^{\top}}.$$

We first apply Sherman-Morrison to  $(\mathbf{X}_{S_{-i}}^{\top} \mathbf{X}_{S_{-i}})^{-1} = (\mathbf{X}_S^{\top} \mathbf{X}_S - \mathbf{x}_i \mathbf{x}_i^{\top})^{-1}$  on the r.h.s. of the above:

$$\sum_i \frac{1 - \mathbf{x}_i^{\top} (\mathbf{X}_S^{\top} \mathbf{X}_S)^{-1} \mathbf{x}_i}{s - d} \left( (\mathbf{X}_S^{\top} \mathbf{X}_S)^{-1} + \frac{(\mathbf{X}_S^{\top} \mathbf{X}_S)^{-1} \mathbf{x}_i \mathbf{x}_i^{\top} (\mathbf{X}_S^{\top} \mathbf{X}_S)^{-1}}{1 - \mathbf{x}_i^{\top} (\mathbf{X}_S^{\top} \mathbf{X}_S)^{-1} \mathbf{x}_i} \right) ((\mathbf{I}_S \mathbf{X})^{\top} - \mathbf{x}_i \mathbf{e}_i^{\top}).$$

Next we expand the last two factors into 4 terms. The expectation of the first  $(\mathbf{X}_S^\top \mathbf{X}_S)^{-1} (\mathbf{I}_S \mathbf{X})^\top$  is  $(\mathbf{I}_S \mathbf{X})^\top$  (which is the l.h.s.) and the expectations of the remaining three terms times  $s - d$  sum to 0:

$$\begin{aligned} & - \sum_{i \in S} (1 - \mathbf{x}_i^\top (\mathbf{X}_S^\top \mathbf{X}_S)^{-1} \mathbf{x}_i) (\mathbf{X}_S^\top \mathbf{X}_S)^{-1} \mathbf{x}_i \mathbf{e}_i^\top + \cancel{(\mathbf{X}_S^\top \mathbf{X}_S)^{-1} \sum_{i \notin S} \mathbf{x}_i \mathbf{x}_i^\top (\mathbf{X}_S^\top \mathbf{X}_S)^{-1} (\mathbf{I}_S \mathbf{X})^\top} \\ & - \sum_{i \in S} (\mathbf{X}_S^\top \mathbf{X}_S)^{-1} \mathbf{x}_i (\mathbf{x}_i^\top (\mathbf{X}_S^\top \mathbf{X}_S)^{-1} \mathbf{x}_i) \mathbf{e}_i^\top = 0. \quad \blacksquare \end{aligned}$$

In Appendix B we give an alternate proof using a derivative argument.

**Proof of Theorem 6** Choose  $\mathbf{F}(S) = \frac{s-d+1}{n-d+1} (\mathbf{X}_S^\top \mathbf{X}_S)^{-1}$ . By Lemma 1 it suffices to show  $\mathbf{F}(S) = \sum_{i \in S} P(S_{-i}|S) \mathbf{F}(S_{-i})$  for volume sampling:

$$\frac{s-d+1}{n-d+1} (\mathbf{X}_S^\top \mathbf{X}_S)^{-1} = \sum_{i \in S} \frac{1 - \mathbf{x}_i^\top (\mathbf{X}_S^\top \mathbf{X}_S)^{-1} \mathbf{x}_i}{s-d} \frac{s-d}{n-d+1} (\mathbf{X}_{S_{-i}}^\top \mathbf{X}_{S_{-i}})^{-1}.$$

To show this we apply Sherman-Morrison to  $(\mathbf{X}_{S_{-i}}^\top \mathbf{X}_{S_{-i}})^{-1}$  on the r.h.s.:

$$\begin{aligned} & \sum_{i \in S} (1 - \mathbf{x}_i^\top (\mathbf{X}_S^\top \mathbf{X}_S)^{-1} \mathbf{x}_i) \left( (\mathbf{X}_S^\top \mathbf{X}_S)^{-1} + \frac{(\mathbf{X}_S^\top \mathbf{X}_S)^{-1} \mathbf{x}_i \mathbf{x}_i^\top (\mathbf{X}_S^\top \mathbf{X}_S)^{-1}}{1 - \mathbf{x}_i^\top (\mathbf{X}_S^\top \mathbf{X}_S)^{-1} \mathbf{x}_i} \right) \\ & = (s-d) (\mathbf{X}_S^\top \mathbf{X}_S)^{-1} + \cancel{(\mathbf{X}_S^\top \mathbf{X}_S)^{-1} \sum_{i \notin S} \mathbf{x}_i \mathbf{x}_i^\top (\mathbf{X}_S^\top \mathbf{X}_S)^{-1}} = (s-d+1) (\mathbf{X}_S^\top \mathbf{X}_S)^{-1}. \end{aligned}$$

If some denominators  $1 - \mathbf{x}_i^\top (\mathbf{X}_S^\top \mathbf{X}_S)^{-1} \mathbf{x}_i$  are zero, then we only sum over  $i$  for which the denominators are positive. In this case the above matrix equality becomes a positive-definite inequality  $\preceq$ .  $\blacksquare$

### 3. Linear Regression with Smallest Number of Responses

Our main motivation for studying volume sampling came from asking the following simple question. Suppose we want to solve a  $d$ -dimensional linear regression problem with an input matrix  $\mathbf{X}$  of  $n$  rows in  $\mathbb{R}^d$  and a response vector  $\mathbf{y} \in \mathbb{R}^n$ , i.e. find  $\mathbf{w} \in \mathbb{R}^d$  that minimizes the least squares loss  $\|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$  on all  $n$  rows. We use  $L(\mathbf{w})$  to denote this loss. The optimal weight vector minimizes  $L(\mathbf{w})$ , i.e.

$$\mathbf{w}^* \stackrel{\text{def}}{=} \operatorname{argmin}_{\mathbf{w} \in \mathbb{R}^d} L(\mathbf{w}) = \mathbf{X}^+ \mathbf{y}.$$

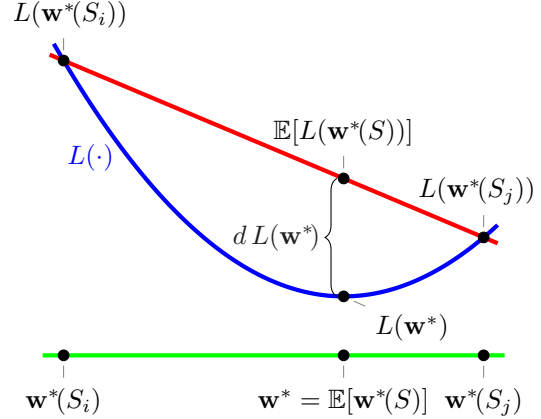
Computing it requires access to the input matrix  $\mathbf{X}$  and the response vector  $\mathbf{y}$ . Assume we are given  $\mathbf{X}$  but the access to response vector  $\mathbf{y}$  is restricted. We are allowed to pick a random subset  $S \subseteq \{1..n\}$  of fixed size  $s$  for which the responses  $\mathbf{y}_S$  for the submatrix  $\mathbf{X}_S$  are revealed to us, and then must produce a weight vector  $\mathbf{w}(\mathbf{X}, S, \mathbf{y}_S) \in \mathbb{R}^d$  from a subset of row indices  $S$  of the input matrix  $\mathbf{X}$  and the corresponding responses  $\mathbf{y}_S$ . Our goal in this paper is to find a distribution on the subsets  $S$  of size  $s$  and a *weight function*  $\mathbf{w}(\mathbf{X}, S, \mathbf{y}_S)$  s.t.<sup>6</sup>

$$\forall (\mathbf{X}, \mathbf{y}) \in \mathbb{R}^{n \times d} \times \mathbb{R}^{n \times 1} : \mathbb{E}[L(\mathbf{w}(\mathbf{X}, S, \mathbf{y}_S))] \leq (1+c) L(\mathbf{w}^*),$$

6. Since the learner is given  $\mathbf{X}$ , it is natural to define the optimal multiplicative constant specialized for each  $\mathbf{X}$ :  $c_{\mathbf{X},s} = \min_c \min_{P(\cdot), \mathbf{w}(\cdot)} \max_{\mathbf{y}} \mathbb{E}_P[L(\mathbf{w}(\mathbf{X}, S, \mathbf{y}_S))] \leq (1+c) L(\mathbf{w}^*)$ , where the domain for distribution  $P(\cdot)$  and weight function  $\mathbf{w}(\cdot)$  are sets of size  $s$ . Showing specialized bounds for  $c_{\mathbf{X},s}$  is left for future research.

where  $c$  must be a fixed constant (that is independent of  $\mathbf{X}$  and  $\mathbf{y}$ ). Throughout the paper we use the one argument shorthand  $\mathbf{w}(S)$  for the weight function  $\mathbf{w}(\mathbf{X}, S, \mathbf{y}_S)$ . We assume that attaining response values is expensive and ask the question: What is the smallest number of responses (i.e. smallest size of  $S$ ) for which such a multiplicative bound is possible? We will use volume sampling to show that attaining  $d$  response values is sufficient and show that less than  $d$  responses is not.

Before we state our main upper bound based on volume sampling, we make the following key observation: If for the subproblem  $(\mathbf{X}_S, \mathbf{y}_S)$  there is a weight vector  $\mathbf{w}(S)$  that has loss zero, then the algorithm has to predict with such a consistent weight vector. This is because in that case the responses  $\mathbf{y}_S$  can be extended to a response vector  $\mathbf{y}$  for all of  $\mathbf{X}$  s.t.  $L(\mathbf{w}^*) = 0$ . Thus since we aim for a multiplicative loss bound, we force the algorithm to predict with the optimum solution  $\mathbf{w}^*(S) \stackrel{\text{def}}{=} (\mathbf{X}_S)^+ \mathbf{y}_S$  whenever the subproblem  $(\mathbf{X}_S, \mathbf{y}_S)$  has loss 0. In particular, when  $|S| = d$  and  $\mathbf{X}_S$  has full rank, then there is a unique consistent solution  $\mathbf{w}^*(S)$  for the subproblem and the learner must use the weight function  $\mathbf{w}(S) = \mathbf{w}^*(S)$ .



**Figure 4:** Unbiased estimator  $\mathbf{w}^*(S)$  in expectation suffers loss  $(d + 1) L(\mathbf{w}^*)$ .

**Theorem 8** *If the input matrix  $\mathbf{X} \in \mathbb{R}^{n \times d}$  is in general position, then for any response vector  $\mathbf{y} \in \mathbb{R}^n$ , the expected square loss (on all  $n$  rows of  $\mathbf{X}$ ) of the optimal solution  $\mathbf{w}^*(S)$  for the subproblem  $(\mathbf{X}_S, \mathbf{y}_S)$ , with the  $d$ -element set  $S$  obtained from volume sampling, is given by*

$$\mathbb{E}[L(\mathbf{w}^*(S))] = (d + 1) L(\mathbf{w}^*).$$

*If  $\mathbf{X}$  is not in general position, then the expected loss is upper-bounded by  $(d + 1) L(\mathbf{w}^*)$ .*

There are no range restrictions on the  $n$  points and response values in this bound. Also, as discussed in the introduction, this bound is already non-obvious for dimension 1, when the multiplicative factor is 2 (See Figure 1 for a visualization). Note that if there is a bias term in dimension 1, then the factor becomes 3.

In dimension  $d$ , it is instructive to look at the case when the square loss of the optimum solution is zero, i.e. there is a weight vector  $\mathbf{w}^* \in \mathbb{R}^d$  s.t.  $\mathbf{X}\mathbf{w}^* = \mathbf{y}$ . In this case the response values of any  $d$  linearly independent rows of  $\mathbf{X}$  determine the optimum solution and the multiplicative loss formula of the theorem clearly holds. The formula specifies how noise-free case generalizes gracefully to the noisy case in that for volume sampling, the expected square loss of the solution obtained from  $d$  row response pairs is always by a factor of at most  $d + 1$  larger than the square loss of the optimum solution. Moreover, since  $\mathbb{E}[\mathbf{w}^*(S)] = \mathbf{w}^*$  and the loss function  $L(\cdot)$  is convex, we have by Jensen's inequality that

$$\mathbb{E}[L(\mathbf{w}^*(S))] \geq L(\mathbb{E}[\mathbf{w}^*(S)]) = L(\mathbf{w}^*).$$

The above theorem now states that the gap  $\mathbb{E}[L(\mathbf{w}^*(S))] - L(\mathbf{w}^*)$  in Jensen's inequality (which coincides with the "regret" of the estimator) equals  $d L(\mathbf{w}^*)$ , when the expectation is w.r.t. size  $d$  volume sampling and  $\mathbf{X}$  is in general position (See Figure 4 for a schematic). As we will show in Section 3.4, this gap also equals the variance  $\mathbb{E}[\|\mathbf{X}\mathbf{w}^*(S) - \mathbf{X}\mathbf{w}^*\|^2]$  of the predictions since the estimator is unbiased. In summary:

$$\underbrace{\mathbb{E}[L(\mathbf{w}^*(S))] - L(\mathbf{w}^*)}_{\text{regret}} = \underbrace{d L(\mathbf{w}^*)}_{\text{gap in Jensen's}} = \underbrace{\mathbb{E}[\|\mathbf{X}\mathbf{w}^*(S) - \mathbf{X}\mathbf{w}^*\|^2]}_{\text{variance}}.$$

We now make a number of observations and present some lower bounds that highlight the upper bound of the above theorem. Then, in Section 3.3 we prove the theorem and a matrix expectation formula implied by it.

### 3.1 When $\mathbf{X}$ is not in General Position

The above theorem gives an equality for the expected loss of a volume-sampled solution. However, this equality is only guaranteed to hold when matrix  $\mathbf{X}$  is in general position. We give a minimal example problem where the matrix  $\mathbf{X}$  is not in general position and the equality of Theorem 8 turns into a strict inequality. This shows that for the equality, the general position assumption is necessary. If we apply even an infinitesimal additive perturbation to the matrix  $\mathbf{X}$  of the example problem, then the resulting matrix  $\mathbf{X}_\epsilon$  is in general position and the equality holds. Note that even though the optimum loss  $L(\mathbf{w}^*)$  does not change significantly under such a perturbation, the expected sampling loss  $\mathbb{E}[L(\mathbf{w}^*(S))]$  has to jump sufficiently to close the gap in the inequality. In our minimal example problem,  $n = 3$  and  $d = 2$ , and

$$\mathbf{X} = \begin{pmatrix} 1 & 1 \\ 1 & 1 \\ 1 & 0 \end{pmatrix}, \quad \mathbf{y} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}.$$

We have three 2-element subsets to sample from:  $S_1 = \{1, 2\}$ ,  $S_2 = \{2, 3\}$ ,  $S_3 = \{1, 3\}$ . Notice that the first two rows of  $\mathbf{X}$  are identical, which means that the probability of sampling set  $S_1$  is 0 in the volume sampling process. The other two subsets,  $S_2$  and  $S_3$ , form identical submatrices  $\mathbf{X}_{S_2} = \mathbf{X}_{S_3}$ . Therefore they are equally probable. The optimal weight vectors for these sets are  $\mathbf{w}^*(S_2) = (0, 0)^\top$  and  $\mathbf{w}^*(S_3) = (0, 1)^\top$ . Also  $\mathbf{w}^* = (0, \frac{1}{2})^\top$  and the expected loss is bounded as:

$$\mathbb{E}[L(\mathbf{w}^*(S))] = \underbrace{\frac{1}{2} L(\mathbf{w}^*(S_2)) + \frac{1}{2} L(\mathbf{w}^*(S_3))}_1 < \underbrace{\frac{3}{(d+1)} L(\mathbf{w}^*)}_{3/2}.$$

Now consider a slightly perturbed input matrix

$$\mathbf{X}_\epsilon = \begin{pmatrix} 1 & 1 + \epsilon \\ 1 & 1 \\ 1 & 0 \end{pmatrix},$$

where  $\epsilon > 0$  is arbitrarily small (We keep the response vector  $\mathbf{y}$  the same). Now, there is no  $d \times d$  submatrix that is singular, so the upper bound from Theorem 8 must be tight. The reason is that even though subset  $S_1$  still has very small probability, its loss is very large, so the expectation is significantly affected by this component, no matter how small  $\epsilon$  is. We see this directly in the calculations. Let  $\mathbf{w}^*$  and  $\mathbf{w}^*(S_i)$  be the corresponding solutions for the perturbed problem and its subproblems. The volumes of the subproblems and their losses are:

$$\begin{aligned} \det(\mathbf{X}_{S_1}^\top \mathbf{X}_{S_1}) &= \epsilon^2 & L(\mathbf{w}^*(S_1)) &= \epsilon^{-2} \\ \det(\mathbf{X}_{S_2}^\top \mathbf{X}_{S_2}) &= 1 & L(\mathbf{w}^*(S_2)) &= 1 \\ \det(\mathbf{X}_{S_3}^\top \mathbf{X}_{S_3}) &= (1 + \epsilon)^2 & L(\mathbf{w}^*(S_3)) &= (1 + \epsilon)^{-2} \end{aligned} \quad L(\mathbf{w}^*) = \frac{1}{2(1 + \epsilon + \epsilon^2)}.$$

Note that for each subproblem, the product of volume times loss is equal to 1. Now the expected loss can be easily computed, and we can see that the gap in the bound disappears (the denominator is the normalizing constant for volume sampling):

$$\mathbb{E}[L(\mathbf{w}^*(S))] = \frac{1 + 1 + 1}{\epsilon^2 + 1 + (1 + \epsilon)^2} = (d + 1) L(\mathbf{w}^*).$$

### 3.2 Lower Bounds and the Importance of Joint Sampling

The factor  $d + 1$  in Theorem 8 cannot, in general, be improved when selecting only  $d$  responses:

**Proposition 9** *For any  $d$ , there exists a least squares problem  $(\mathbf{X}, \mathbf{y})$  with  $d + 1$  rows in  $\mathbb{R}^d$  such that for every  $d$ -element index set  $S \subseteq \{1 \dots d + 1\}$ , we have*

$$L(\mathbf{w}^*(S)) = (d + 1) L(\mathbf{w}^*).$$

**Proof** Choose the input vectors  $\mathbf{x}_i$  (and rows  $\mathbf{x}_i^\top$ ) as the  $d + 1$  corners of any simplex in  $\mathbb{R}^d$  centered at the origin and choose all  $d + 1$  responses as the same non-zero value  $\alpha$ . For any  $\alpha$ , the optimal solution  $\mathbf{w}^*$  will be the all-zeros vector with loss

$$L(\mathbf{w}^*) = (d + 1) \alpha^2.$$

On the other hand, taking any size  $d$  subset of indices  $S \subseteq \{1 \dots d + 1\}$ , the subproblem solution  $\mathbf{w}^*(S)$  will only produce loss on the left out input vector  $\mathbf{x}_i$ , indexed with  $i \notin S$ . To obtain the prediction on  $x_i$ , we use a simple geometric argument. Observe that since the simplex is centered, we can write the origin of  $\mathbb{R}^d$  in terms of the corners of the simplex as

$$\mathbf{0} = \sum_k \mathbf{x}_k = \mathbf{x}_i + d \bar{\mathbf{x}}_{-i}, \quad \text{where } \bar{\mathbf{x}}_{-i} \stackrel{\text{def}}{=} \frac{1}{d} \sum_{k \neq i} \mathbf{x}_k.$$

Thus, the left out input vector  $\mathbf{x}_i$  equals  $-d \bar{\mathbf{x}}_{-i}$ . The prediction of  $\mathbf{w}^*(S)$  on this vector is

$$\hat{y}_i = \mathbf{x}_i^\top \mathbf{w}^*(S) = -d \left( \frac{1}{d} \sum_{k \neq i} \mathbf{x}_k^\top \right) \mathbf{w}^*(S) = - \sum_{k \neq i} \mathbf{x}_k^\top \mathbf{w}^*(S) = -d\alpha.$$

It follows that the loss of  $\mathbf{w}^*(S)$  equals

$$L(\mathbf{w}^*(S)) = (\hat{y}_i - y_i)^2 = (-d\alpha - \alpha)^2 = (d + 1)^2 \alpha^2 = (d + 1) L(\mathbf{w}^*). \quad \blacksquare$$

Moreover, it is easy to show that no *deterministic* algorithm for selecting  $d$  rows (without knowing the responses) can guarantee a multiplicative loss bound with a factor less than  $n/d$  (Boutsidis et al., 2013). For the sake of completeness, we show this here for  $d = 1$ :

**Proposition 10** *For any  $n \times 1$  input matrix  $\mathbf{X}$  of all 1's and any deterministic algorithm that chooses some singleton set  $S = \{i\}$ , there is a response vector  $\mathbf{y}$  for which the loss of the subproblem and the optimal loss are related as follows:*

$$L(\mathbf{w}^*(S)) = n L(\mathbf{w}^*).$$

**Proof** If the response vector  $\mathbf{y}$  is the vector of  $n$  1's except for a single 0 at index  $i$ , then we have

$$L(\underbrace{\mathbf{w}^*(\{i\})}_{n-1}) = n L(\underbrace{\mathbf{w}^*}_{\frac{n-1}{n}}). \quad \blacksquare$$

Note that for the 1-dimensional example used in the proof, volume sampling would pick the set  $S$  uniformly. For this distribution, the multiplicative factor drops from  $n$  down to 2, that is  $\mathbb{E}[L(\mathbf{w}^*(S))] = \frac{1}{n}(n-1) + \frac{n-1}{n}1 = 2 L(\mathbf{w}^*)$ .

*The importance of joint sampling.* Three properties of volume sampling play a crucial role in achieving a multiplicative loss bound:

- a) *Randomness.* No deterministic algorithm guarantees such a bound (see Proposition 10).
- b) *The chosen submatrices must have full rank.* Choosing any rank deficient submatrix with positive probability, does not allow for a multiplicative bound (see Propositions 11 and 12).
- c) *Jointness.* No i.i.d. sampling procedure can achieve a multiplicative loss bound with  $O(d)$  responses (see Corollary 13).

By jointly selecting subset  $S$ , volume sampling ensures that the corresponding input vectors  $\mathbf{x}_i$  are well spread out in the input space  $\mathbb{R}^d$ . In particular, volume sampling does not put any probability mass on sets  $S$  such that the rank of submatrix  $\mathbf{X}_S$  is less than  $d$ . Intuitively, selecting rank deficient row subsets should not be effective, since such a choice leads to an under-determined least squares problem. We make this simple statement more precise by showing that any randomized algorithm, that with positive probability selects a rank deficient row subset, cannot achieve a multiplicative loss bound. Intuitively if the algorithm picks a rank deficient subset then it is not clear how it should select the weight vector  $\mathbf{w}(S)$  given input matrix  $\mathbf{X}$ , subset  $S$  and responses  $\mathbf{y}_S$ . We reasoned before that  $\mathbf{w}(S)$  must have loss 0 on the subproblem  $(\mathbf{X}_S, \mathbf{y}_S)$ . However if  $\text{rank}(\mathbf{X}_S) < d$ , then the choice of the weight vector  $\mathbf{w}(S)$  with loss 0 is not unique and this causes positive loss for some response vector  $\mathbf{y}$ .

**Proposition 11** *If for any input matrix  $\mathbf{X}$ , the algorithm samples a rank deficient subset  $S$  of rows with positive probability, then the expected loss of the algorithm cannot be bounded by a constant times the optimum loss for all response vectors  $\mathbf{y}$ .*

Note that this means in particular that if  $\mathbf{X}$  has rank  $d$ , then sampling  $d-1$  size subsets with positive probability does not allow for a constant factor approximation.

**Proof** Let  $S$  be a rank deficient subset chosen with probability  $P(S) > 0$ . Since in our setup the bound has to hold for all response vectors  $\mathbf{y}$  we can imagine an adversary choosing a worst-case  $\mathbf{y}$ . This adversary gives all rows of  $\mathbf{X}_S$  the response value zero. Let  $\mathbf{w}(S)$  be the plane produced by the algorithm when choosing  $S$  and receiving the responses 0 for  $\mathbf{X}_S$ . Let  $i \in \{1..n\}$  s.t.  $\mathbf{x}_i^\top \notin \text{row-span}(\mathbf{X}_S)$  and let  $\mathbf{w}^*$  be any weight vector that gives response value 0 to all rows of  $\mathbf{X}_S$  and response value  $\mathbf{x}_i^\top \mathbf{w}(S) + Y$  to  $\mathbf{x}_i$ . The adversary chooses  $\mathbf{y}$  as  $\mathbf{X}\mathbf{w}^*$ , i.e. it gives all points  $\mathbf{x}_j$  not indexed by  $S$  and different from  $\mathbf{x}_i$  the response values  $\mathbf{x}_j^\top \mathbf{w}^*$  as well. Now  $\mathbf{w}^*$  has total loss 0 but  $\mathbf{w}(S)$  has loss  $Y^2$  on  $\mathbf{x}_i$  and the algorithm's expected total loss is  $\geq P(S) Y^2$ .  $\blacksquare$



We now strengthen the above proposition in that whenever the sample  $S$  is rank deficient then the loss of the optimum is zero while the loss of the algorithm is positive. However note that this proposition is weaker than the above in that it only holds for specific input matrices.

**Proposition 12** *Let  $d \leq n$  and let  $\mathbf{X}$  be any input matrix of rank  $d$  consisting of  $n$  standard basis row vectors in  $\mathbb{R}^d$ . Then for any randomized learning algorithm that with probability  $p$  selects a subset  $S$  s.t.  $\text{rank}(\mathbf{X}_S) < d$  and any weight function  $\mathbf{w}(\cdot)$ , there is a response vector  $\mathbf{y}$ , satisfying:*

$$L(\mathbf{w}^*) = 0, \quad \text{and} \quad L(\mathbf{w}(S)) > 0 \quad \text{with probability at least } p.$$

**Proof** Let  $Q = \{1, 2, \dots, 2^n\}$ . The adversarial response vector  $\mathbf{y}$  is constructed by carefully selecting one of the weight vectors  $\mathbf{w}^* \in Q^d$ , and setting the response vector  $\mathbf{y}$  to  $\mathbf{X}\mathbf{w}^*$ . This ensures that  $L(\mathbf{w}^*) = 0$  and since  $\mathbf{X}$  consists of standard basis row vectors, the components of  $\mathbf{y}$  lie in  $Q$  as well. Note that if the learner does not discover  $\mathbf{w}^*$  exactly, it will incur positive loss. Let  $\mathcal{H}$  be the set of all rank deficient sets in  $\mathbf{X}$ , i.e. those that lack at least one of the standard basis vectors:

$$\mathcal{H} = \{S \subseteq \{1..n\} : \text{rank}(\mathbf{X}_S) < d\}.$$

Suppose that given matrix  $\mathbf{X}$ , the learner uses weight function  $\mathbf{w}(S, \mathbf{y}_S)$ . (Note that for the sake of concreteness we stopped using the single argument shorthand for the weight function during this proof.) We will count the number of possible inputs to this function, when  $S$  is a rank deficient index set of the rows of  $\mathbf{X}$  and the response vector  $\mathbf{y}_S$  is consistent with some  $\mathbf{w}^* \in Q^d$ . For any fixed rank deficient set  $S$ , let  $t$  be the number of distinct basis vectors appearing in  $\mathbf{X}_S$ . Clearly  $t \leq d - 1$ . Fix a subset  $T \subseteq S$  of size  $t$  s.t.  $\mathbf{X}_T$  contains all  $t$  basis vectors of  $\mathbf{X}_S$  exactly once (Thus the basis vectors in  $\mathbf{X}_{S \setminus T}$  are all duplicates). Since  $\mathbf{y} \in Q^n$ , the components of  $\mathbf{y}_S$  also lie in  $Q$  and  $\mathbf{y}_S$  is determined by the responses of  $\mathbf{y}_T$ . Clearly there are at most  $|Q|^{d-1}$  choices for  $\mathbf{y}_T$ . It follows that the number of possible input pairs  $(S, \mathbf{y}_S)$  for function  $\mathbf{w}(\cdot, \cdot)$  under the above restrictions can be bounded as

$$\begin{aligned} \left| \left\{ (S, \mathbf{y}_S) : [S \in \mathcal{H}] \text{ and } [\mathbf{y}_S = \mathbf{X}_S \mathbf{w}^* \text{ for } \mathbf{w}^* \in Q^d] \right\} \right| &\leq \underbrace{|\mathcal{H}|}_{< 2^n} \underbrace{\max_{S \in \mathcal{H}} |\{\mathbf{X}_S \mathbf{w}^* : \mathbf{w}^* \in Q^d\}|}_{\leq |Q|^{d-1}} \\ &< 2^n |Q|^{d-1} = |Q|^d. \end{aligned}$$

So for every weight function  $\mathbf{w}(\cdot, \cdot)$ , there exists  $\mathbf{w}^* \in Q^d$  that is not present in the set  $\{\mathbf{w}(S, \mathbf{y}_S) : S \in \mathcal{H}\}$ . Selecting  $\mathbf{y} = \mathbf{X}\mathbf{w}^*$  for the adversarial response vector, we guarantee that the learner picks the wrong solution for every rank deficient set  $S$  and therefore receives positive loss w.p. at least  $p$ . ■

Using Proposition 12, we show that any i.i.d. row sampling distribution (like for example leverage score sampling) requires  $\Omega(d \log d)$  samples to get any multiplicative loss bound, either with high probability or in expectation.

**Corollary 13** *Let  $d \leq n$  and let  $\mathbf{X}$  be any input matrix of rank  $d$  consisting of  $n$  standard basis row vectors in  $\mathbb{R}^d$ . Then for any randomized learning algorithm which selects a random multiset  $S \subseteq \{1..n\}$  of size  $|S| \leq (d - 1) \ln(d)$  via i.i.d. sampling from any distribution and uses any weight function  $\mathbf{w}(S)$ , there is a response vector  $\mathbf{y}$  satisfying:*

$$L(\mathbf{w}^*) = 0, \quad \text{and} \quad L(\mathbf{w}(S)) > 0 \quad \text{with probability at least } 1/2.$$

**Proof** Any i.i.d. sample of size at most  $(d - 1) \ln(d)$  with probability at least  $1/2$  does not contain all of the unique standard basis vectors (Coupon Collector Problem<sup>7</sup>). Thus, with probability at least  $1/2$  submatrix  $\mathbf{X}_S$  has rank less than  $d$ . Now, for any such algorithm we can use Proposition 12 to select a consistent adversarial response vector  $\mathbf{y}$  such that with probability at least  $1/2$  the loss  $L(\mathbf{w}(S))$  is positive. ■

Note that the corollary requires  $\mathbf{X}$  to be of a restricted form that contains a lot of duplicate rows. It is open whether this corollary still holds when  $\mathbf{X}$  is an arbitrary full rank matrix.

### 3.3 Proof of the Loss Expectation Formula

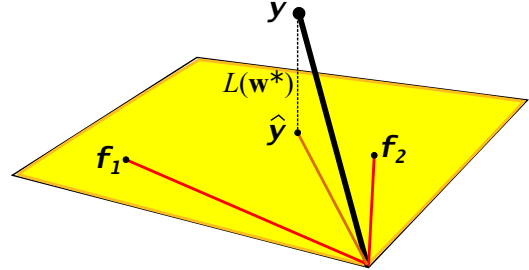
First, we discuss several key connections between linear regression and volume, which are used in the proof. Note that the loss  $L(\mathbf{w}^*)$  suffered by the optimum weight vector can be written as  $\|\hat{\mathbf{y}} - \mathbf{y}\|^2$ , the squared Euclidean distance between prediction vector  $\hat{\mathbf{y}} = \mathbf{X}\mathbf{w}^*$  and the response vector  $\mathbf{y}$ . Since  $\hat{\mathbf{y}}$  is minimizing the distance from  $\mathbf{y}$  to the subspace of  $\mathbb{R}^n$  spanning the feature vectors  $\{\mathbf{f}_1, \dots, \mathbf{f}_d\}$  (columns of  $\mathbf{X}$ ), it has to be the *projection* of  $\mathbf{y}$  onto that subspace (see Figure 5). We denote this projection as  $\mathbf{P}_{\mathbf{X}} \mathbf{y}$ , as defined in Section 2.2. Note that  $\mathbf{P}_{\mathbf{X}}$  is a linear mapping from  $\mathbb{R}^n$  onto the column span of the matrix  $\mathbf{X}$  such that

$$\text{for } \mathbf{u} \in \text{span}(\mathbf{X}) \quad \mathbf{u} = \mathbf{P}_{\mathbf{X}} \mathbf{y} \Leftrightarrow \mathbf{P}_{\mathbf{X}} (\mathbf{u} - \mathbf{y}) = \mathbf{0} \Leftrightarrow \mathbf{X}^\top (\mathbf{u} - \mathbf{y}) = \mathbf{0}. \quad (4)$$

We next give a second geometric interpretation of the length  $\|\hat{\mathbf{y}} - \mathbf{y}\|^2$ . Let  $\mathcal{P}$  be the parallelepiped formed by the  $d$  column/feature vectors of the input matrix  $\mathbf{X}$ . Furthermore, consider the extended input matrix produced by adding the response vector  $\mathbf{y}$  to  $\mathbf{X}$  as an extra column:

$$\tilde{\mathbf{X}} \stackrel{\text{def}}{=} (\mathbf{X}, \mathbf{y}) \in \mathbb{R}^{n \times (d+1)}. \quad (5)$$

Using the “base  $\times$  height” formula we can relate the volume of  $\mathcal{P}$  to the volume of  $\tilde{\mathcal{P}}$ , the parallelepiped formed by the  $d + 1$  columns of  $\tilde{\mathbf{X}}$ . Observe that  $\tilde{\mathcal{P}}$  has  $\mathcal{P}$  as one of its faces, with the response vector  $\mathbf{y}$  representing the edge that protrudes from that face. Hence the volume of  $\tilde{\mathcal{P}}$  is the product of the volume of  $\mathcal{P}$  and the distance between  $\mathbf{y}$  and  $\text{span}(\mathbf{X})$ . This distance equals  $\|\hat{\mathbf{y}} - \mathbf{y}\|$ , since as discussed above,  $\hat{\mathbf{y}}$  is the projection of  $\mathbf{y}$  onto  $\text{span}(\mathbf{X})$ . Thus we have



**Figure 5:** Prediction vector  $\hat{\mathbf{y}}$  is a projection of  $\mathbf{y}$  onto the span of feature vectors  $\mathbf{f}_i$ .

$$\det(\tilde{\mathbf{X}}^\top \tilde{\mathbf{X}}) = \det(\mathbf{X}^\top \mathbf{X}) L(\mathbf{w}^*). \quad (6)$$

Next, we present a proposition whose corollary is key to proving Theorem 8. Suppose that we select one test row from the input matrix and use the remaining  $n - 1$  row response pairs as the training set. The proposition relates the loss of the obtained solution on the test row to the total leave-one-out loss on all rows.

**Proposition 14** *For any index  $i \in \{1..n\}$ , let  $\mathbf{w}^{*(-i)}$  be the solution to the reduced linear regression problem  $(\mathbf{X}_{-i}, \mathbf{y}_{-i})$ . Then*

7. This was proven for uniform sampling in Theorem 1.24 of Auger and Doerr (2011). It can be shown that uniform sampling is the best case for Coupon Collector Problem (Holst, 2001), so the bound holds for any i.i.d. sampling.

$$L(\mathbf{w}^*(-i)) - L(\mathbf{w}^*) = \underbrace{\frac{\det(\mathbf{X}^\top \mathbf{X}) - \det(\mathbf{X}_{-i}^\top \mathbf{X}_{-i})}{\det(\mathbf{X}^\top \mathbf{X})}}_{\mathbf{x}_i^\top (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{x}_i} \ell_i(\mathbf{w}^*(-i)),$$

where  $\ell_i(\mathbf{w}) \stackrel{\text{def}}{=} (\mathbf{x}_i^\top \mathbf{w} - y_i)^2$  is the square loss of  $\mathbf{w}$  on the  $i$ -th point.

An algebraic proof of this proposition essentially appears in the proof of Theorem 11.7 in Cesa-Bianchi and Lugosi (2006). For the sake of completeness we give a new geometric proof of this proposition in Appendix C using basic properties of volume, thus stressing the connection to volume sampling.

Note that if matrix  $\mathbf{X}$  has exactly  $n = d + 1$  rows and the training matrix  $\mathbf{X}_{-i}$  is full rank, then  $\mathbf{w}^*(-i)$  has loss zero on all training rows. In this case we obtain a simpler relationship than the proposition.

**Corollary 15** *If  $\mathbf{X}$  has  $d + 1$  rows and  $\text{rank}(\mathbf{X}_{-i}) = d$ , then defining  $\tilde{\mathbf{X}}$  as in (5), we have*

$$\det(\tilde{\mathbf{X}}^\top \tilde{\mathbf{X}}) = \det(\mathbf{X}_{-i}^\top \mathbf{X}_{-i}) \ell_i(\mathbf{w}^*(-i)).$$

**Proof** By Proposition 14 and the fact that  $L(\mathbf{w}^*(-i)) = \ell_i(\mathbf{w}^*(-i))$ , we have

$$\det(\mathbf{X}^\top \mathbf{X}) L(\mathbf{w}^*) = \det(\mathbf{X}_{-i}^\top \mathbf{X}_{-i}) \ell_i(\mathbf{w}^*(-i)).$$

The corollary now follows from the “base  $\times$  height” formula for volume. ■

We are now ready to present the proof of Theorem 8. Recall that our goal is to find the expected loss  $\mathbb{E}[L(\mathbf{w}^*(S))]$ , where  $S$  is a size  $d$  volume sampled set.

**Proof of Theorem 8** First, we rewrite the expectation as follows:

$$\begin{aligned} \mathbb{E}[L(\mathbf{w}^*(S))] &= \sum_{S, |S|=d} P(S) L(\mathbf{w}^*(S)) = \sum_{S, |S|=d} P(S) \sum_{j=1}^n \ell_j(\mathbf{w}^*(S)) \\ &= \sum_{S, |S|=d} \sum_{j \notin S} P(S) \ell_j(\mathbf{w}^*(S)) = \sum_{T, |T|=d+1} \sum_{j \in T} P(T_{-j}) \ell_j(\mathbf{w}^*(T_{-j})). \end{aligned} \quad (7)$$

We now use Corollary 15 on the matrix  $\mathbf{X}_T$  and test row  $\mathbf{x}_j^\top$  (assuming  $\text{rank}(\mathbf{X}_{T_{-j}}) = d$ ):

$$P(T_{-j}) \ell_j(\mathbf{w}^*(T_{-j})) = \frac{\det(\mathbf{X}_{T_{-j}}^\top \mathbf{X}_{T_{-j}})}{\det(\mathbf{X}^\top \mathbf{X})} \ell_j(\mathbf{w}^*(T_{-j})) = \frac{\det(\tilde{\mathbf{X}}_T^\top \tilde{\mathbf{X}}_T)}{\det(\mathbf{X}^\top \mathbf{X})}. \quad (8)$$

Since the summand does not depend on the index  $j \in T$ , the inner summation in (7) becomes a multiplication by  $d + 1$ . This lets us write the expected loss as:

$$\mathbb{E}[L(\mathbf{w}^*(S))] = \frac{d + 1}{\det(\mathbf{X}^\top \mathbf{X})} \sum_{T, |T|=d+1} \det(\tilde{\mathbf{X}}_T^\top \tilde{\mathbf{X}}_T) \stackrel{(1)}{=} (d + 1) \frac{\det(\tilde{\mathbf{X}}^\top \tilde{\mathbf{X}})}{\det(\mathbf{X}^\top \mathbf{X})} \stackrel{(2)}{=} (d + 1) L(\mathbf{w}^*), \quad (9)$$

where (1) follows from the Cauchy-Binet formula and (2) is an application of the “base  $\times$  height” formula. If  $\mathbf{X}$  is not in general position, then for some summands in (8),  $\text{rank}(\mathbf{X}_{T_{-j}}) < d$  and

$P(T_{-j}) = 0$ . Thus the left-hand side of (8) is 0, while the right-hand side is non-negative, so (9) becomes an inequality, completing the proof of Theorem 8.  $\blacksquare$

*Lifting expectations to matrix form.* We can now show the matrix expectation formula of Theorem 7 as a corollary to the loss expectation formula of Theorem 8. The key observation is that the loss formula holds for arbitrary response vector  $\mathbf{y}$ , which allows us to “lift” it to the matrix form.

**Proof of Theorem 7** Note, that the loss of least squares estimator can be written in terms of the projection matrix  $\mathbf{P}_{\mathbf{X}}$ :

$$L(\mathbf{w}^*) = \|\mathbf{y} - \hat{\mathbf{y}}\|^2 = \|(\mathbf{I} - \mathbf{P}_{\mathbf{X}})\mathbf{y}\|^2 = \mathbf{y}^\top (\mathbf{I} - \mathbf{P}_{\mathbf{X}})^2 \mathbf{y} \stackrel{(*)}{=} \mathbf{y}^\top (\mathbf{I} - \mathbf{P}_{\mathbf{X}}) \mathbf{y},$$

where in  $(*)$  we used the following property of a projection matrix:  $\mathbf{P}_{\mathbf{X}}^2 = \mathbf{P}_{\mathbf{X}}$ . Writing the loss expectation of the subsampled estimator in the same form, we obtain:

$$\begin{aligned} \mathbb{E}[L(\mathbf{w}^*(S))] &= \mathbb{E}[\|\mathbf{y} - \hat{\mathbf{y}}(S)\|^2] = \mathbb{E}[\|(\mathbf{I} - \mathbf{X}(\mathbf{I}_S \mathbf{X})^+) \mathbf{y}\|^2] \\ &= \mathbb{E}[\mathbf{y}^\top (\mathbf{I} - \mathbf{X}(\mathbf{I}_S \mathbf{X})^+)^2 \mathbf{y}] = \mathbf{y}^\top \mathbb{E}[(\mathbf{I} - \mathbf{X}(\mathbf{I}_S \mathbf{X})^+)^2] \mathbf{y}. \end{aligned}$$

Crucially, we are able to extract the response vector  $\mathbf{y}$  out of the expectation formula, which allows us to write the formula from Theorem 8 as follows:

$$\mathbf{y}^\top \mathbb{E}[(\mathbf{I} - \mathbf{X}(\mathbf{I}_S \mathbf{X})^+)^2] \mathbf{y} = \mathbf{y}^\top (d+1)(\mathbf{I} - \mathbf{P}_{\mathbf{X}}) \mathbf{y}, \quad \forall \mathbf{y} \in \mathbb{R}^n.$$

We now use the following elementary fact: If for two symmetric matrices  $\mathbf{A}$  and  $\mathbf{B}$ , we have  $\mathbf{y}^\top \mathbf{A} \mathbf{y} = \mathbf{y}^\top \mathbf{B} \mathbf{y}$ ,  $\forall \mathbf{y} \in \mathbb{R}^n$ , then  $\mathbf{A} = \mathbf{B}$ .<sup>8</sup> This gives the matrix expectation formula:

$$\mathbb{E}[(\mathbf{I} - \mathbf{X}(\mathbf{I}_S \mathbf{X})^+)^2] = (d+1)(\mathbf{I} - \mathbf{P}_{\mathbf{X}}).$$

Expanding square on the l.h.s. of the above and applying Theorem 5, we obtain the covariance-type equivalent form stated in Theorem 7:

$$\begin{aligned} \mathbf{I} - 2 \overbrace{\mathbb{E}[\mathbf{X}(\mathbf{I}_S \mathbf{X})^+]}^{\mathbf{P}_{\mathbf{X}}} + \mathbb{E}[(\mathbf{X}(\mathbf{I}_S \mathbf{X})^+)^2] &= (d+1)(\mathbf{I} - \mathbf{P}_{\mathbf{X}}) \\ \iff \mathbb{E}[(\mathbf{X}(\mathbf{I}_S \mathbf{X})^+)^2] - \mathbf{P}_{\mathbf{X}} &= d(\mathbf{I} - \mathbf{P}_{\mathbf{X}}). \end{aligned} \quad \blacksquare$$

### 3.4 Averaging Unbiased Estimators and the Open Problem for Worst-case Responses

As discussed at the beginning of Section 3, our goal is to find a way to sample a small index set  $S$  and construct a weight function  $\mathbf{w}(S)$  which uses responses  $\mathbf{y}_S$  so that  $\mathbb{E}[L(\mathbf{w}(S))] \leq (1+c)L(\mathbf{w}^*)$ , where the multiplicative factor  $1+c$  is bounded for all input matrices  $\mathbf{X}$  and all response vectors  $\mathbf{y}$ . Recall that  $L(\cdot)$  denotes the square loss on all rows and  $\mathbf{w}^*$  is the optimal solution based on all responses. We show in the previous subsections that the smallest size of  $S$  for which this goal can be achieved is  $d$  (There is no sampling procedure for sets of size less than  $d$  and weight function  $\mathbf{w}(S)$  for which this factor is finite). We also prove that when sets  $S$  of size  $d$  are drawn proportional to

8. Similarly, if  $\mathbf{y}^\top \mathbf{A} \mathbf{y} \leq \mathbf{y}^\top \mathbf{B} \mathbf{y}$ ,  $\forall \mathbf{y} \in \mathbb{R}^n$ , then the positive-definite inequality  $\mathbf{A} \preceq \mathbf{B}$  holds for the matrices.

the squared volume of  $\mathbf{X}_S$  (i.e.  $\det(\mathbf{X}_S^\top \mathbf{X}_S)$ ), then  $\mathbb{E}[L(\mathbf{w}^*(S))] \leq (d+1)L(\mathbf{w}^*)$ , where the factor  $d+1$  is optimal for some  $\mathbf{X}$  and  $\mathbf{y}$ . Here  $\mathbf{w}^*(S)$  denotes the linear least squares solution for the subproblem  $(\mathbf{X}_S, \mathbf{y}_S)$ .

A natural more general goal is to get arbitrarily close to the optimum loss. That is, for any  $\epsilon$ , what is the smallest sample size  $|S| = s$  for which there is a sampling distribution over subsets  $S$  and a weight function  $\mathbf{w}(S)$  built from  $\mathbf{X}$  and  $\mathbf{y}_S$ , such that  $\mathbb{E}[L(\mathbf{w}(S))] \leq (1+\epsilon)L(\mathbf{w}^*)$ . A related bound for i.i.d. leverage score sampling states that a sample size of  $O(d \log d + \frac{d}{\epsilon})$  suffices to achieve a  $1+\epsilon$  factor *with high probability* (Hsu, 2017; Dereziński, 2018), however this does not imply multiplicative bounds *in expectation*.<sup>9</sup>

We conjecture that some form of volume sampling can be used to achieve the  $1+\epsilon$  factor with sample size  $O(\frac{d}{\epsilon})$ , in expectation. How close can we get with the techniques presented in this paper? We showed that size  $d$  volume sampling achieves a factor of  $1+d$ , but we do not know how to generalize this proof to sample size larger than  $d$ . However, one unique property of the volume-sampled estimator  $\mathbf{w}^*(S)$  that can be useful here is that it is an *unbiased estimator* of  $\mathbf{w}^*$ . As we shall see now, this basic property has many benefits. For any unbiased estimator (i.e.  $\mathbb{E}[\mathbf{w}(S)] = \mathbf{w}^*$ ) and optimal prediction vector  $\hat{\mathbf{y}} = \mathbf{X}\mathbf{w}^*$ , consider the following rudimentary version of a bias-variance decomposition:

$$\underbrace{\mathbb{E} \|\mathbf{X} \mathbf{w}(S) - \mathbf{y}\|^2}_{L(\mathbf{w}(S))} = \mathbb{E} \|\mathbf{X} \mathbf{w}(S) - \hat{\mathbf{y}} + \hat{\mathbf{y}} - \mathbf{y}\|^2 = \mathbb{E} \|\mathbf{X} \mathbf{w}(S) - \hat{\mathbf{y}}\|^2 + \underbrace{\|\hat{\mathbf{y}} - \mathbf{y}\|^2}_{L(\mathbf{w}^*)}. \quad (10)$$

The unbiasedness of the estimator assures that the cross term  $(\mathbf{X} \overbrace{\mathbb{E}[\mathbf{w}(S)]}^{\mathbf{w}^*} - \hat{\mathbf{y}})^\top (\hat{\mathbf{y}} - \mathbf{y})$  is 0. Therefore a  $1+c$  factor loss bound is equivalent to a  $c$  factor variance bound, i.e.

$$\underbrace{\mathbb{E}[L(\mathbf{w}(S))] \leq (1+c)L(\mathbf{w}^*)}_{\text{loss bound}} \iff \underbrace{\mathbb{E} \|\mathbf{X} \mathbf{w}(S) - \hat{\mathbf{y}}\|^2 \leq cL(\mathbf{w}^*)}_{\text{variance bound}}. \quad (11)$$

To reduce the variance of any unbiased estimator  $\mathbf{w}(S)$  (i.e.  $\mathbb{E}[\mathbf{w}(S)] = \mathbf{w}^*$ ) with sample size  $s$ , we can draw  $k$  independent samples  $S_1, \dots, S_k$  of size  $s$  each and predict with the average estimator  $\frac{1}{k} \sum_{j=1}^k \mathbf{w}(S_j)$ . If the loss bound from (11) holds for  $\mathbf{w}(S)$ , then the average estimator satisfies

$$\mathbb{E} \left[ L \left( \frac{1}{k} \sum_j \mathbf{w}(S_j) \right) \right] \leq \left( 1 + \frac{c}{k} \right) L(\mathbf{w}^*).$$

Setting  $k = c/\epsilon$ , we need  $t = sc/\epsilon$  responses to get a  $1+\epsilon$  approximation. We showed that size  $s = d$  volume sampling achieves factor  $c = d$ . So with our current proof techniques, we need  $t = d^2/\epsilon$  responses to get a  $1+\epsilon$  factor approximation, for  $\epsilon \in (0, d]$ .<sup>10</sup>

9. Also, the weight vectors produced from i.i.d. leverage score sampling are not unbiased.

10. Thus when averaging the estimators of  $k = t/d$  independent volume sampled sets of size  $d$ ,

$$\underbrace{\mathbb{E} \left[ L \left( \frac{1}{k} \sum_j \mathbf{w}^*(S_j) \right) \right]}_{\text{regret}} - L(\mathbf{w}^*) = \underbrace{\frac{d^2 L(\mathbf{w}^*)}{t}}_{\text{prediction variance}}, \quad \text{when } \mathbf{X} \text{ is in general position.}$$

The basic open problem for worst-case responses is the following: Is there a size  $O(d/\epsilon)$  unbiased estimator that achieves a  $1 + \epsilon$  factor approximation?<sup>11</sup> By the above averaging method this is equivalent to the following question: Is there a size  $O(d)$  unbiased estimator that achieves a constant factor? This is because once we have an unbiased estimator that achieves a constant factor, then by averaging  $1/\epsilon$  copies, we get the  $1 + O(\epsilon)$  factor. Ideally the special unbiased estimators resulting from a version of volume sampling can achieve this feat. We conclude this section with our favorite open problem: Is there a version of  $O(d)$  size volume sampling that achieves a constant factor approximation?

In the next section we make some minimal statistical assumptions on the response vector which let us prove much stronger bounds: We assume that the response vector is linear plus bounded noise of mean zero. In particular we show that with this noise model,  $O(d)$  size volume sampling achieves a constant factor approximation.

#### 4. Regularized Volume Sampling for Learning with Noisy Responses

Volume sampling, as defined in Section 2.1, has certain fundamental limitations. Namely, it is undefined whenever matrix  $\mathbf{X}$  is not full rank or if we wish to sample a subset  $S$  of size smaller than the dimension  $d$ . Motivated by these limitations, we propose a regularized variant, called  $\lambda$ -regularized volume sampling, which we define through a generalization of the reverse iterative sampling procedure:

$$P(S_{-i} | S) \propto \frac{\det(\mathbf{X}_{S_{-i}}^\top \mathbf{X}_{S_{-i}} + \lambda \mathbf{I})}{\det(\mathbf{X}_S^\top \mathbf{X}_S + \lambda \mathbf{I})}. \quad (12)$$

---

##### Algorithm 1 $\lambda$ -regularized v. sampling

---

```

 $S \leftarrow \{1..n\}$ 
while  $|S| > s$ 
   $\forall_{i \in S}: h_i \leftarrow \frac{\det(\mathbf{X}_{S_{-i}}^\top \mathbf{X}_{S_{-i}} + \lambda \mathbf{I})}{\det(\mathbf{X}_S^\top \mathbf{X}_S + \lambda \mathbf{I})}$ 
  Sample  $i \propto h_i$  out of  $S$ 
   $S \leftarrow S - \{i\}$ 
end
return  $S$ 

```

---

The normalization factor of this conditional probability (i.e. the sum of (12) over  $i \in S$ ) can be computed using Sylvester's theorem:

$$\begin{aligned} \sum_{i \in S} \frac{\det(\mathbf{X}_{S_{-i}}^\top \mathbf{X}_{S_{-i}} + \lambda \mathbf{I})}{\det(\mathbf{X}_S^\top \mathbf{X}_S + \lambda \mathbf{I})} &= \sum_{i \in S} (1 - \mathbf{x}_i^\top (\mathbf{X}_S^\top \mathbf{X}_S + \lambda \mathbf{I})^{-1} \mathbf{x}_i) \\ &= |S| - \text{tr}(\mathbf{X}_S (\mathbf{X}_S^\top \mathbf{X}_S + \lambda \mathbf{I})^{-1} \mathbf{X}_S^\top) \\ &= |S| - d + \lambda \text{tr}((\mathbf{X}_S^\top \mathbf{X}_S + \lambda \mathbf{I})^{-1}). \end{aligned} \quad (13)$$

Note that in the special case of no regularization (i.e.  $\lambda = 0$ ) the last trace vanishes and (13) is equal to  $|S| - d$ , so we recover volume sampling from Section 2.1. However, when  $\lambda > 0$ , then the last term is non-zero and depends on the entire matrix  $\mathbf{X}_S$ . This makes regularized volume sampling more complicated and certain equalities proven in previous sections for  $\lambda = 0$  no longer hold. In particular, the analogous closed form of the sampling probability  $P(S)$  given in Theorem 2 is not recovered because the paths from node  $\{1..n\}$  to node  $S$  in the graph of Figure 3 do not all have the same probability. However, the proof technique we developed for reverse iterative sampling can still be applied, resulting in the following extension of the variance formula of Theorem 6:

---

11. In a recent paper (Chen and Price, 2017) a  $1 + \epsilon$  factor approximation has been achieved with  $O(d/\epsilon)$  examples (for  $\epsilon \in (0, 1]$ ), but the guarantee holds with high probability (and not in expectation) and the estimator is not unbiased.

**Theorem 16** For any  $\mathbf{X} \in \mathbb{R}^{n \times d}$ ,  $\lambda \geq 0$ , let  $S$  be sampled according to  $\lambda$ -regularized size  $s$  volume sampling from  $\mathbf{X}$ . Then,

$$\mathbb{E}[(\mathbf{X}_S^\top \mathbf{X}_S + \lambda \mathbf{I})^{-1}] \preceq \frac{n - d_\lambda + 1}{s - d_\lambda + 1} (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1}$$

for any  $s \geq d_\lambda \stackrel{\text{def}}{=} \text{tr}(\mathbf{X}(\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^\top)$ .

Constant  $d_\lambda$  is a common notion of statistical dimension often referred to as the effective degrees of freedom. If  $\lambda_i$  are the eigenvalues of  $\mathbf{X}^\top \mathbf{X}$ , then  $d_\lambda = \sum_{i=1}^d \frac{\lambda_i}{\lambda_i + \lambda}$ . Note that  $d_\lambda$  is decreasing with  $\lambda$  and, when  $\mathbf{X}$  is full rank,  $d_0 = d$ . Thus, unlike Theorem 6, the above result offers meaningful bounds for sampling sets  $S$  of size smaller than  $d$ .

**Proof** To obtain Theorem 16, we use essentially the same methodology as described in Lemma 1, except in the regularized case equality is replaced with inequality. Recall that using Sylvester's theorem we can compute the unnormalized conditional probability from (12) as:

$$h_i = \frac{\det(\mathbf{X}_{S-i}^\top \mathbf{X}_{S-i} + \lambda \mathbf{I})}{\det(\mathbf{X}_S^\top \mathbf{X}_S + \lambda \mathbf{I})} = 1 - \mathbf{x}_i^\top (\mathbf{X}_S^\top \mathbf{X}_S + \lambda \mathbf{I})^{-1} \mathbf{x}_i.$$

From now on, we will use  $\mathbf{Z}_\lambda(S) = \mathbf{X}_S^\top \mathbf{X}_S + \lambda \mathbf{I}$  as a shorthand in the proofs. Next, letting  $M = \sum_{i \in S} h_i$ , we compute unnormalized expectation by applying the Sherman-Morrison formula:

$$\begin{aligned} M \mathbb{E}[(\mathbf{X}_{S-i}^\top \mathbf{X}_{S-i} + \lambda \mathbf{I})^{-1} | S] &= \sum_{i \in S} h_i \mathbf{Z}_\lambda(S-i)^{-1} = \sum_{i \in S} h_i \left( \mathbf{Z}_\lambda(S)^{-1} + \frac{\mathbf{Z}_\lambda(S)^{-1} \mathbf{x}_i \mathbf{x}_i^\top \mathbf{Z}_\lambda(S)^{-1}}{1 - \mathbf{x}_i^\top \mathbf{Z}_\lambda(S)^{-1} \mathbf{x}_i} \right) \\ &= M \mathbf{Z}_\lambda(S)^{-1} + \mathbf{Z}_\lambda(S)^{-1} \left( \sum_{i \in S} \mathbf{x}_i \mathbf{x}_i^\top \right) \mathbf{Z}_\lambda(S)^{-1} \\ &= M \mathbf{Z}_\lambda(S)^{-1} + \mathbf{Z}_\lambda(S)^{-1} (\mathbf{Z}_\lambda(S) - \lambda \mathbf{I}) \mathbf{Z}_\lambda(S)^{-1} \\ &= M \mathbf{Z}_\lambda(S)^{-1} + \mathbf{Z}_\lambda(S)^{-1} - \lambda \mathbf{Z}_\lambda(S)^{-2} \\ &\preceq (M + 1) \mathbf{Z}_\lambda(S)^{-1}. \end{aligned}$$

Finally, the normalization factor  $M$  (which we already computed in (13)) can be lower-bounded using the  $\lambda$ -statistical dimension  $d_\lambda$  of matrix  $\mathbf{X}$ :

$$M = \sum_{i \in S} (1 - \mathbf{x}_i^\top \mathbf{Z}_\lambda(S)^{-1} \mathbf{x}_i) = s - d + \lambda \text{tr}(\mathbf{Z}_\lambda(S)^{-1}) \geq s - \underbrace{(d - \lambda \text{tr}(\mathbf{Z}_\lambda(\{1..n\})^{-1}))}_{d_\lambda}.$$

Putting the bounds together, we obtain that:

$$\mathbb{E}[(\mathbf{X}_{S-i}^\top \mathbf{X}_{S-i} + \lambda \mathbf{I})^{-1} | S] \preceq \frac{s - d_\lambda + 1}{s - d_\lambda} (\mathbf{X}_S^\top \mathbf{X}_S + \lambda \mathbf{I})^{-1}.$$

To prove Theorem 16 it remains to chain the conditional expectations along the sequence of subsets obtained by  $\lambda$ -regularized volume sampling:

$$\mathbb{E}[\mathbf{Z}_\lambda(S)^{-1}] \preceq \left( \prod_{t=s+1}^n \frac{t - d_\lambda + 1}{t - d_\lambda} \right) \mathbf{Z}_\lambda(\{1..n\})^{-1} = \frac{n - d_\lambda + 1}{s - d_\lambda + 1} (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1}. \quad \blacksquare$$

#### 4.1 Ridge Regression with Noisy Responses

We apply the above result to obtain statistical guarantees for subsampling with regularized estimators. Given a matrix  $\mathbf{X} \in \mathbb{R}^{n \times d}$ , we consider the task of fitting a linear model to a vector of responses  $\mathbf{y} = \mathbf{X}\tilde{\mathbf{w}} + \boldsymbol{\xi}$ , where  $\tilde{\mathbf{w}} \in \mathbb{R}^d$  and the noise  $\boldsymbol{\xi} \in \mathbb{R}^n$  is a mean zero random vector with covariance matrix  $\text{Var}[\boldsymbol{\xi}] \preceq \sigma^2 \mathbf{I}$  for some  $\sigma > 0$ . A classical solution to this task is the ridge estimator:

$$\mathbf{w}_\lambda^* = \underset{\mathbf{w} \in \mathbb{R}^d}{\text{argmin}} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 + \lambda \|\mathbf{w}\|^2 = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{y}.$$

As a consequence of Theorem 16, we show that if  $S$  is sampled with  $\lambda$ -regularized volume sampling from  $\mathbf{X}$ , then the ridge estimator for the subproblem  $(\mathbf{X}_S, \mathbf{y}_S)$

$$\mathbf{w}_{\lambda}^*(S) = (\mathbf{X}_S^\top \mathbf{X}_S + \lambda \mathbf{I})^{-1} \mathbf{X}_S^\top \mathbf{y}_S$$

has strong generalization properties with respect to the full problem  $(\mathbf{X}, \mathbf{y})$  in terms of the mean squared prediction error (MSPE) and mean squared error (MSE).

**Theorem 17** *Let  $\mathbf{X} \in \mathbb{R}^{n \times d}$  and  $\tilde{\mathbf{w}} \in \mathbb{R}^d$ , and suppose that  $\mathbf{y} = \mathbf{X}\tilde{\mathbf{w}} + \boldsymbol{\xi}$ , where  $\boldsymbol{\xi}$  is a mean zero vector with  $\text{Var}[\boldsymbol{\xi}] \preceq \sigma^2 \mathbf{I}$ . Let  $S$  be sampled according to  $\lambda$ -regularized size  $s \geq d_\lambda$  volume sampling from  $\mathbf{X}$  and  $\mathbf{w}_\lambda^*(S)$  be the  $\lambda$ -ridge estimator of  $\tilde{\mathbf{w}}$  computed from subproblem  $(\mathbf{X}_S, \mathbf{y}_S)$ . Then, if  $\lambda \leq \frac{\sigma^2}{\|\tilde{\mathbf{w}}\|^2}$ , we have*

$$\begin{aligned} \text{(mean squared prediction error)} \quad \mathbb{E}_S \mathbb{E}_\xi \left[ \frac{1}{n} \|\mathbf{X}(\mathbf{w}_\lambda^*(S) - \tilde{\mathbf{w}})\|^2 \right] &\leq \frac{\sigma^2 d_\lambda}{s - d_\lambda + 1}, \\ \text{(mean squared error)} \quad \mathbb{E}_S \mathbb{E}_\xi \left[ \|\mathbf{w}_\lambda^*(S) - \tilde{\mathbf{w}}\|^2 \right] &\leq \frac{\sigma^2 n \text{tr}((\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1})}{s - d_\lambda + 1}. \end{aligned}$$

Next, we present two lower bounds for MSPE of a subsampled ridge estimator which show that the statistical guarantees achieved by regularized volume sampling are nearly optimal for  $s \gg d_\lambda$  and better than standard approaches for  $s = O(d_\lambda)$ . In particular, we show that non-i.i.d. nature of volume sampling is essential if we want to achieve good generalization when the number of responses is close to  $d_\lambda$ . Namely for certain data matrices, any i.i.d. subsampling procedure (such as i.i.d. leverage score sampling) requires at least  $d_\lambda \ln(d_\lambda)$  responses to achieve MSPE below  $\sigma^2$ . In contrast volume sampling obtains that bound for any matrix with  $2d_\lambda$  responses.

**Theorem 18** *For any  $p \geq 1$  and  $\sigma \geq 0$ , there is  $d \geq p$  such that for any sufficiently large  $n$  divisible by  $d$ , there exists a matrix  $\mathbf{X} \in \mathbb{R}^{n \times d}$  such that*

$$d_\lambda(\mathbf{X}) \geq p \quad \text{for any } 0 \leq \lambda \leq \sigma^2,$$

and for each of the following two statements there is a vector  $\tilde{\mathbf{w}} \in \mathbb{R}^d$  for which the corresponding regression problem  $\mathbf{y} = \mathbf{X}\tilde{\mathbf{w}} + \boldsymbol{\xi}$  with  $\text{Var}[\boldsymbol{\xi}] = \sigma^2 \mathbf{I}$  satisfies that statement:

a) For any subset  $S \subseteq \{1..n\}$  of size  $s$ ,

$$\mathbb{E}_\xi \left[ \frac{1}{n} \|\mathbf{X}(\mathbf{w}_\lambda^*(S) - \tilde{\mathbf{w}})\|^2 \right] \geq \frac{\sigma^2 d_\lambda}{s + d_\lambda};$$



b) For multiset  $S \subseteq \{1..n\}$  of size  $s \leq (d_\lambda - 1) \ln(d_\lambda)$ , sampled i.i.d. from any distribution over  $\{1..n\}$ ,

$$\mathbb{E}_S \mathbb{E}_\xi \left[ \frac{1}{n} \|\mathbf{X}(\mathbf{w}_\lambda^*(S) - \tilde{\mathbf{w}})\|^2 \right] \geq \sigma^2.$$

**Proof of Theorem 17** Standard analysis for the ridge regression estimator follows by performing bias-variance decomposition of the error, and then selecting  $\lambda$  so that bias can be appropriately bounded. We will recall this calculation for a fixed subproblem  $(\mathbf{X}_S, \mathbf{y}_S)$ . First, we compute the bias of the ridge estimator for a fixed set  $S$  (recall the shorthand  $\mathbf{Z}_\lambda(S) = \mathbf{X}_S^\top \mathbf{X}_S + \lambda \mathbf{I}$ ):

$$\begin{aligned} \text{Bias}_\xi[\mathbf{w}_\lambda^*(S)] &= \mathbb{E}[\mathbf{w}_\lambda^*(S)] - \tilde{\mathbf{w}} = \mathbb{E}_\xi [\mathbf{Z}_\lambda(S)^{-1} \mathbf{X}_S^\top \mathbf{y}_S] - \tilde{\mathbf{w}} \\ &= \mathbf{Z}_\lambda(S)^{-1} \mathbf{X}_S^\top (\mathbf{X}_S \tilde{\mathbf{w}} + \mathbb{E}_\xi[\boldsymbol{\xi}_S]) - \tilde{\mathbf{w}} \\ &= (\mathbf{Z}_\lambda(S)^{-1} \mathbf{X}_S^\top \mathbf{X}_S - \mathbf{I}) \tilde{\mathbf{w}} = -\lambda \mathbf{Z}_\lambda(S)^{-1} \tilde{\mathbf{w}}. \end{aligned}$$

Similarly, the covariance matrix of  $\mathbf{w}_\lambda^*(S)$  is given by:

$$\begin{aligned} \text{Var}_\xi[\mathbf{w}_\lambda^*(S)] &= \mathbf{Z}_\lambda(S)^{-1} \mathbf{X}_S^\top \text{Var}_\xi[\boldsymbol{\xi}_S] \mathbf{X}_S \mathbf{Z}_\lambda(S)^{-1} \\ &\leq \sigma^2 \mathbf{Z}_\lambda(S)^{-1} \mathbf{X}_S^\top \mathbf{X}_S \mathbf{Z}_\lambda(S)^{-1} = \sigma^2 (\mathbf{Z}_\lambda(S)^{-1} - \lambda \mathbf{Z}_\lambda(S)^{-2}). \end{aligned}$$

Mean squared error of the ridge estimator for a fixed subset  $S$  can now be bounded by:

$$\begin{aligned} \mathbb{E}_\xi [\|\mathbf{w}_\lambda^*(S) - \tilde{\mathbf{w}}\|^2] &= \text{tr}(\text{Var}_\xi[\mathbf{w}_\lambda^*(S)]) + \|\text{Bias}_\xi[\mathbf{w}_\lambda^*(S)]\|^2 \\ &\leq \sigma^2 \text{tr}(\mathbf{Z}_\lambda(S)^{-1} - \lambda \mathbf{Z}_\lambda(S)^{-2}) + \lambda^2 \text{tr}(\mathbf{Z}_\lambda(S)^{-2} \tilde{\mathbf{w}} \tilde{\mathbf{w}}^\top) \\ &\leq \sigma^2 \text{tr}(\mathbf{Z}_\lambda(S)^{-1}) + \lambda \text{tr}(\mathbf{Z}_\lambda(S)^{-2}) (\lambda \|\tilde{\mathbf{w}}\|^2 - \sigma^2) \tag{14} \\ &\leq \sigma^2 \text{tr}(\mathbf{Z}_\lambda(S)^{-1}), \tag{15} \end{aligned}$$

where in (14) we applied Cauchy-Schwartz inequality for matrix trace, and in (15) we used the assumption that  $\lambda \leq \frac{\sigma^2}{\|\tilde{\mathbf{w}}\|^2}$ . Thus, taking expectation over the sampling of set  $S$ , we get

$$\begin{aligned} \mathbb{E}_S \mathbb{E}_\xi [\|\mathbf{w}_\lambda^*(S) - \tilde{\mathbf{w}}\|^2] &\leq \sigma^2 \mathbb{E}_S [\text{tr}(\mathbf{Z}_\lambda(S)^{-1})] \\ \text{(Theorem 16)} \quad &\leq \sigma^2 \frac{n - d_\lambda + 1}{s - d_\lambda + 1} \text{tr}(\mathbf{Z}_\lambda(\{1..n\})^{-1}) \tag{16} \\ &\leq \frac{\sigma^2 n \text{tr}((\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1})}{s - d_\lambda + 1}. \end{aligned}$$

Next, we bound the mean squared prediction error. As before, we start with the standard bias-variance decomposition for fixed set  $S$ :

$$\begin{aligned} \mathbb{E}_\xi [\|\mathbf{X}(\mathbf{w}_\lambda^*(S) - \tilde{\mathbf{w}})\|^2] &= \text{tr}(\text{Var}_\xi[\mathbf{X} \mathbf{w}_\lambda^*(S)]) + \|\mathbf{X}(\mathbb{E}_\xi[\mathbf{w}_\lambda^*(S)] - \tilde{\mathbf{w}})\|^2 \\ &\leq \sigma^2 \text{tr}(\mathbf{X}(\mathbf{Z}_\lambda(S)^{-1} - \lambda \mathbf{Z}_\lambda(S)^{-2}) \mathbf{X}^\top) + \lambda^2 \text{tr}(\mathbf{Z}_\lambda(S)^{-1} \mathbf{X}^\top \mathbf{X} \mathbf{Z}_\lambda(S)^{-1} \tilde{\mathbf{w}} \tilde{\mathbf{w}}^\top) \\ &\leq \sigma^2 \text{tr}(\mathbf{X} \mathbf{Z}_\lambda(S)^{-1} \mathbf{X}^\top) + \lambda \text{tr}(\mathbf{X} \mathbf{Z}_\lambda(S)^{-2} \mathbf{X}^\top) (\lambda \|\tilde{\mathbf{w}}\|^2 - \sigma^2) \\ &\leq \sigma^2 \text{tr}(\mathbf{X} \mathbf{Z}_\lambda(S)^{-1} \mathbf{X}^\top). \end{aligned}$$

Once again, taking expectation over subset  $S$ , we have

$$\begin{aligned} \mathbb{E}_S \mathbb{E}_\xi \left[ \frac{1}{n} \|\mathbf{X}(\mathbf{w}_\lambda^*(S) - \tilde{\mathbf{w}})\|^2 \right] &\leq \frac{\sigma^2}{n} \mathbb{E}_S [\text{tr}(\mathbf{X} \mathbf{Z}_\lambda(S)^{-1} \mathbf{X}^\top)] = \frac{\sigma^2}{n} \text{tr}(\mathbf{X} \mathbb{E}_S [\mathbf{Z}_\lambda(S)^{-1}] \mathbf{X}^\top) \\ \text{(Theorem 16)} \quad &\leq \frac{\sigma^2}{n} \frac{n - d_\lambda + 1}{s - d_\lambda + 1} \text{tr}(\mathbf{X} \mathbf{Z}_\lambda(\{1..n\})^{-1} \mathbf{X}^\top) \leq \frac{\sigma^2 d_\lambda}{s - d_\lambda + 1}. \end{aligned} \quad (17)$$

The key part of proving both bounds is the application of Theorem 16. For MSE, we only used the trace version of the inequality (see (16)), however to obtain the bound on MSPE we used the more general positive semi-definite inequality in (17).  $\blacksquare$

**Proof of Theorem 18** Let  $d = \lceil p \rceil + 1$  and  $n \geq \lceil \sigma^2 \rceil d(d-1)$  be divisible by  $d$ . We define

$$\mathbf{X} \stackrel{\text{def}}{=} [\mathbf{I}, \dots, \mathbf{I}]^\top \in \mathbb{R}^{n \times d}, \quad \tilde{\mathbf{w}}^\top \stackrel{\text{def}}{=} [a\sigma, \dots, a\sigma] \in \mathbb{R}^d$$

for some  $a > 0$ . For any  $\lambda \leq \sigma^2$ , the  $\lambda$ -statistical dimension of  $\mathbf{X}$  is

$$d_\lambda = \text{tr}(\mathbf{X} \mathbf{Z}_\lambda(\{1..n\})^{-1} \mathbf{X}^\top) \geq \frac{\lceil \sigma^2 \rceil d(d-1)}{\lceil \sigma^2 \rceil (d-1) + \lambda} \geq \frac{d(d-1)}{d-1+1} \geq p.$$

Let  $S \subseteq \{1..n\}$  be any set of size  $s$ , and for  $i \in \{1..d\}$  let  $s_i \stackrel{\text{def}}{=} |\{i \in S : \mathbf{x}_i = \mathbf{e}_i\}|$ . The prediction variance of estimator  $\mathbf{w}_\lambda^*(S)$  is equal to

$$\begin{aligned} \text{tr}(\text{Var}_\xi[\mathbf{X} \mathbf{w}_\lambda^*(S)]) &= \sigma^2 \text{tr}(\mathbf{X}(\mathbf{Z}_\lambda(S)^{-1} - \lambda \mathbf{Z}_\lambda(S)^{-2}) \mathbf{X}^\top) \\ &= \frac{\sigma^2 n}{d} \sum_{i=1}^d \left( \frac{1}{s_i + \lambda} - \frac{\lambda}{(s_i + \lambda)^2} \right) = \frac{\sigma^2 n}{d} \sum_{i=1}^d \frac{s_i}{(s_i + \lambda)^2}. \end{aligned}$$

The prediction bias of estimator  $\mathbf{w}_\lambda^*(S)$  is equal to

$$\begin{aligned} \|\mathbf{X}(\mathbb{E}_\xi[\mathbf{w}_\lambda^*(S)] - \tilde{\mathbf{w}})\|^2 &= \lambda^2 \tilde{\mathbf{w}}^\top \mathbf{Z}_\lambda(S)^{-1} \mathbf{X}^\top \mathbf{X} \mathbf{Z}_\lambda(S)^{-1} \tilde{\mathbf{w}} \\ &= \frac{\lambda^2 a^2 \sigma^2 n}{d} \text{tr}(\mathbf{Z}_\lambda(S)^{-2}) = \frac{\lambda^2 a^2 \sigma^2 n}{d} \sum_{i=1}^d \frac{1}{(s_i + \lambda)^2}. \end{aligned}$$

Thus, MSPE of estimator  $\mathbf{w}_\lambda^*(S)$  is given by:

$$\begin{aligned} \mathbb{E}_\xi \left[ \frac{1}{n} \|\mathbf{X}(\mathbf{w}_\lambda^*(S) - \tilde{\mathbf{w}})\|^2 \right] &= \frac{1}{n} \text{tr}(\text{Var}_\xi[\mathbf{X} \mathbf{w}_\lambda^*(S)]) + \frac{1}{n} \|\mathbf{X}(\mathbb{E}_\xi[\mathbf{w}_\lambda^*(S)] - \tilde{\mathbf{w}})\|^2 \\ &= \frac{\sigma^2}{d} \sum_{i=1}^d \left( \frac{s_i}{(s_i + \lambda)^2} + \frac{a^2 \lambda^2}{(s_i + \lambda)^2} \right) = \frac{\sigma^2}{d} \sum_{i=1}^d \frac{s_i + a^2 \lambda^2}{(s_i + \lambda)^2}. \end{aligned}$$

Next, we find the  $\lambda$  that minimizes this expression. Taking the derivative with respect to  $\lambda$  we get:

$$\frac{\partial}{\partial \lambda} \left( \frac{\sigma^2}{d} \sum_{i=1}^d \frac{s_i + a^2 \lambda^2}{(s_i + \lambda)^2} \right) = \frac{\sigma^2}{d} \sum_{i=1}^d \frac{2s_i(\lambda - a^{-2})}{(s_i + \lambda)^3}.$$

Thus, since at least one  $s_i$  has to be greater than 0, for any set  $S$  the derivative is negative for  $\lambda < a^{-2}$  and positive for  $\lambda > a^{-2}$ , and the unique minimum of MSPE is achieved at  $\lambda = a^{-2}$ , regardless of which subset  $S$  is chosen. So, as we are seeking a lower bound, we can focus on the case of  $\lambda = a^{-2}$ .

*Proof of part a.* Let  $a = 1$ . As shown above, we can assume that  $\lambda = 1$ . In this case the formula simplifies to:

$$\begin{aligned} \mathbb{E}_{\xi} \left[ \frac{1}{n} \|\mathbf{X}(\mathbf{w}_{\lambda}^*(S) - \tilde{\mathbf{w}})\|^2 \right] &= \frac{\sigma^2}{d} \sum_{i=1}^d \frac{s_i + 1}{(s_i + 1)^2} = \frac{\sigma^2}{d} \sum_{i=1}^d \frac{1}{s_i + 1} \\ &\stackrel{(*)}{\geq} \frac{\sigma^2}{\frac{s}{d} + 1} = \frac{\sigma^2 d}{s + d} \geq \frac{\sigma^2 d_{\lambda}}{s + d_{\lambda}}, \end{aligned}$$

where  $(*)$  follows by applying Jensen's inequality to convex function  $\phi(x) = \frac{1}{x+1}$ .

*Proof of part b.* Let  $a = \sqrt{2d}$ . As shown above, we can assume that  $\lambda = 1/(2d)$ . Suppose that multiset  $S$  is sampled i.i.d. from some distribution over set  $\{1..n\}$ . Similarly as in Corollary 13, we exploit the Coupon Collector's problem, i.e. that if  $|S| \leq (d-1) \ln(d)$ , then with probability at least  $1/2$  there is  $i \in \{1..d\}$  such that  $s_i = 0$  (i.e., one of the unit vectors  $\mathbf{e}_i$  was never selected). Thus, MSPE can be lower-bounded as follows:

$$\mathbb{E}_S \mathbb{E}_{\xi} \left[ \frac{1}{n} \|\mathbf{X}(\mathbf{w}_{\lambda}^*(S) - \tilde{\mathbf{w}})\|^2 \right] \geq \frac{1}{2} \frac{\sigma^2}{d} \frac{s_i + a^2 \lambda^2}{(s_i + \lambda)^2} = \frac{\sigma^2}{2d} \frac{2d\lambda^2}{\lambda^2} = \sigma^2. \quad \blacksquare$$

## 5. Efficient Algorithms for Volume Sampling

In this section we propose algorithms for efficiently performing volume sampling. This addresses the question posed by Avron and Boutsidis (2013), asking for a polynomial-time algorithm for the case when the size of set  $S$  is  $s > d$ . Deshpande and Rademacher (2010) gave an algorithm for the case when  $s = d$ , which was later improved by Guruswami and Sinop (2012), running in time  $O(nd^3)$ . Recently, Li et al. (2017) offered an algorithm for arbitrary  $s$ , which has complexity  $O(n^4 s)$ . We propose two new methods, which use our reverse iterative sampling technique to achieve faster running times for volume sampling of any size  $s$ . Both algorithms apply to the more general setting of  $\lambda$ -regularized volume sampling (described in Section 4), and produce standard volume sampling as a special case for  $\lambda = 0$  and  $s \geq d$ . The first algorithm has a deterministic runtime of  $O((n-s+d)nd)$ , whereas the second one is an accelerated version which with high probability finishes in time  $O(nd^2)$ . Thus, we obtain a direct improvement over Li et al. (2017) by a factor of at least  $n^2$ , and in the special case of  $s = d$ , by a factor of  $d$  over the algorithm of Guruswami and Sinop (2012).

Our algorithms implement reverse iterative sampling from Theorem 2. We start with the full index set  $S = \{1..n\}$ . In one step of the algorithm, we remove one row from set  $S$ . After removing  $q$  rows, we are left with the index set of size  $n - q$  that is distributed according to volume sampling for row set size  $n - q$ , and we proceed until our set  $S$  has the desired size  $s$ . The primary cost of the procedure is updating the conditional distribution  $P(S_{-i}|S)$  at every step. It is convenient to store it using the unnormalized weights defined in (12) which, via Sylvester's theorem, can be computed as  $h_i = 1 - \mathbf{x}_i^{\top} (\mathbf{X}_S^{\top} \mathbf{X}_S + \lambda \mathbf{I})^{-1} \mathbf{x}_i$  (For the sake of generality we state the methods for  $\lambda$ -regularized

volume sampling). Doing this naively, we would first compute  $(\mathbf{X}_S^\top \mathbf{X}_S + \lambda \mathbf{I})^{-1}$  which takes  $O(nd^2)$  time<sup>12</sup>. After that for each  $i$ , we would multiply this matrix by  $\mathbf{x}_i$  in time  $O(d^2)$  to get the  $h_i$ 's. The overall runtime of this naive method becomes:

$$\overbrace{\# \text{ of steps}}^{n-s} \times \left( \overbrace{\text{compute } (\mathbf{X}_S^\top \mathbf{X}_S + \lambda \mathbf{I})^{-1}}^{O(nd^2)} + \overbrace{\# \text{ of weights}}^{\leq n} \times \overbrace{\text{compute } h_i}^{O(d^2)} \right) = O((n-s)nd^2).$$

Both the computation of matrix inverse and the weights  $h_i$  can be made more efficient. First, the matrix  $(\mathbf{X}_S^\top \mathbf{X}_S + \lambda \mathbf{I})^{-1}$  can be computed from the one obtained in the previous step by using the Sherman-Morrison formula. This lets us update it in  $O(d^2)$  time instead of  $O(nd^2)$ . Furthermore, we propose two strategies for dealing with the cost of maintaining the weights:

- a) Update all  $h_i$ 's at every step using Sherman-Morrison;
- b) Use rejection sampling and only compute the  $h_i$ 's needed for the rejection trials (This avoids computing all  $h_i$ 's, but makes the computation of each needed  $h_i$  more expensive).

As we can see, there is a trade-off between those strategies. In the following lemma, we will show that updating the value of  $h_i$ , given its value in the previous step only costs  $O(d)$  time as opposed to  $O(d^2)$ . However, the number of  $h_i$ 's that need to be computed for rejection sampling (explained shortly) can be far smaller.

**Lemma 19** *For any matrix  $\mathbf{X} \in \mathbb{R}^{n \times d}$ , set  $S \subseteq \{1..n\}$  and two distinct indices  $i, j \in S$ , we have*

$$1 - \mathbf{x}_j^\top (\mathbf{X}_{S-i}^\top \mathbf{X}_{S-i} + \lambda \mathbf{I})^{-1} \mathbf{x}_j = h_j - (\mathbf{x}_j^\top \mathbf{v})^2,$$

where  $h_j = 1 - \mathbf{x}_j^\top (\mathbf{X}_S^\top \mathbf{X}_S + \lambda \mathbf{I})^{-1} \mathbf{x}_j$  and  $\mathbf{v} = \frac{1}{\sqrt{h_i}} (\mathbf{X}_S^\top \mathbf{X}_S + \lambda \mathbf{I})^{-1} \mathbf{x}_i$ .

**Proof** Letting  $\mathbf{Z}_\lambda(S) = \mathbf{X}_S^\top \mathbf{X}_S + \lambda \mathbf{I}$ , we have

$$\begin{aligned} h_j - (\mathbf{x}_j^\top \mathbf{v})^2 &= 1 - \mathbf{x}_j^\top \mathbf{Z}_\lambda(S)^{-1} \mathbf{x}_j - \frac{(\mathbf{x}_j^\top \mathbf{Z}_\lambda(S)^{-1} \mathbf{x}_i)^2}{1 - \mathbf{x}_i^\top \mathbf{Z}_\lambda(S)^{-1} \mathbf{x}_i} \\ &= 1 - \mathbf{x}_j^\top \mathbf{Z}_\lambda(S)^{-1} \mathbf{x}_j - \frac{\mathbf{x}_j^\top \mathbf{Z}_\lambda(S)^{-1} \mathbf{x}_i \mathbf{x}_i^\top \mathbf{Z}_\lambda(S)^{-1} \mathbf{x}_j}{1 - \mathbf{x}_i^\top \mathbf{Z}_\lambda(S)^{-1} \mathbf{x}_i} \\ &= 1 - \mathbf{x}_j^\top \left( \mathbf{Z}_\lambda(S)^{-1} + \frac{\mathbf{Z}_\lambda(S)^{-1} \mathbf{x}_i \mathbf{x}_i^\top \mathbf{Z}_\lambda(S)^{-1}}{1 - \mathbf{x}_i^\top \mathbf{Z}_\lambda(S)^{-1} \mathbf{x}_i} \right) \mathbf{x}_j \\ &\stackrel{(*)}{=} 1 - \mathbf{x}_j^\top (\mathbf{X}_{S-i}^\top \mathbf{X}_{S-i} + \lambda \mathbf{I})^{-1} \mathbf{x}_j, \end{aligned}$$

where  $(*)$  follows from the Sherman-Morrison formula. ■

Thus the overall time complexity of reverse iterative sampling when using the first strategy goes down by a factor of  $d$  compared to the naive version (except for an initialization cost which stays at  $O(nd^2)$ ).

**Theorem 20** *Algorithm RegVol produces an index set  $S$  of rows distributed according to  $\lambda$ -regularized size  $s$  volume sampling over  $\mathbf{X}$  in time  $O((n-s+d)nd)$ .*

12. We are primarily interested in the case where  $n \geq d$  and we state our time bounds under that assumption. However, when  $\lambda > 0$ , our techniques can be easily adapted to the case of  $n < d$ .

**Proof** Using Lemma 19 for  $h_i$  and the Sherman-Morrison formula for  $\mathbf{Z}$ , the following invariants hold at the beginning of the **while** loop:

$$h_i = 1 - \mathbf{x}_i^\top (\mathbf{X}_S^\top \mathbf{X}_S + \lambda \mathbf{I})^{-1} \mathbf{x}_i \quad \text{and} \quad \mathbf{Z} = (\mathbf{X}_S^\top \mathbf{X}_S + \lambda \mathbf{I})^{-1}.$$

Runtime: Computing the initial  $\mathbf{Z} = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1}$  takes  $O(nd^2)$ , as does computing the initial values of  $h_j$ 's. Inside the **while** loop, updating  $h_j$ 's takes  $O(|S|d) = O(nd)$  and updating  $\mathbf{Z}$  takes  $O(d^2)$ . The overall runtime becomes  $O(nd^2 + (n-s)nd) = O((n-s+d)nd)$ . ■

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**Algorithm 2** RegVol( $\mathbf{X}, s, \lambda$ )
 

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```

1:  $\mathbf{Z} \leftarrow (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1}$ 
2:  $\forall_{i \in \{1..n\}} \quad h_i \leftarrow 1 - \mathbf{x}_i^\top \mathbf{Z} \mathbf{x}_i$ 
3:  $S \leftarrow \{1..n\}$ 
4: while  $|S| > s$ 
5:   Sample  $i \propto h_i$  out of  $S$ 
6:    $S \leftarrow S - \{i\}$ 
7:    $\mathbf{v} \leftarrow \mathbf{Z} \mathbf{x}_i / \sqrt{h_i}$ 
8:    $\forall_{j \in S} \quad h_j \leftarrow h_j - (\mathbf{x}_j^\top \mathbf{v})^2$ 
9:    $\mathbf{Z} \leftarrow \mathbf{Z} + \mathbf{v} \mathbf{v}^\top$ 
10: end
11: return  $S$ 
    
```

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**Algorithm 3** FastRegVol( $\mathbf{X}, s, \lambda$ )
 

---

```

1:  $\mathbf{Z} \leftarrow (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1}$ 
2:  $S \leftarrow \{1..n\}$ 
3: while  $|S| > \max\{s, 2d\}$ 
4:   repeat
5:     Sample  $i$  uniformly out of  $S$ 
6:      $h_i \leftarrow 1 - \mathbf{x}_i^\top \mathbf{Z} \mathbf{x}_i$ 
7:     Sample  $A \sim \text{Bernoulli}(h_i)$ 
8:   until  $A = 1$ 
9:    $S \leftarrow S - \{i\}$ 
10:   $\mathbf{Z} \leftarrow \mathbf{Z} + h_i^{-1} \mathbf{Z} \mathbf{x}_i \mathbf{x}_i^\top \mathbf{Z}$ 
11: end
12: if  $s < 2d$ ,  $S \leftarrow \text{RegVol}(\mathbf{X}_S, s, \lambda)$  end
13: return  $S$ 
    
```

---

Next we present algorithm FastRegVol, which is based on the rejection sampling strategy. Our key observation is that updating the full conditional distribution  $P(S_{-i}|S)$  is wasteful, since the distribution changes very slowly throughout the procedure. Moreover, the unnormalized weights  $h_i$ , which are computed in the process are all bounded by 1. Thus, to sample from the correct distribution at any given iteration, we can employ rejection sampling as follows:

- 1: Sample  $i$  uniformly from set  $S$ ,
- 2: Compute  $h_i$ ,
- 3: Accept with probability  $h_i$ ,
- 4: Otherwise, draw another sample.

Note that this rejection sampling can be employed locally, within each iteration of the algorithm. Thus, one rejection does not revert us back to the beginning of the algorithm. Moreover, if the probability of acceptance is high, then this strategy requires computing only a small number of weights per iteration of the algorithm, as opposed to updating all of them. This turns out to be the case for a majority of the steps of the algorithm, except at the very end (for  $s \leq 2d$ ), where the conditional probabilities start changing more drastically. At that point, it becomes more efficient to use the first algorithm, RegVol.

**Theorem 21** For any  $\lambda, s \geq 0$ , and  $\delta \in (0, 1)$ , algorithm FastRegVol samples according to  $\lambda$ -regularized size  $s$  volume sampling, and with probability at least  $1 - \delta$  runs in time

$$O\left(\left(n + \log(n/d) \log(1/\delta)\right)d^2\right).$$

**Proof** We analyze the efficiency of rejection sampling in FastRegVol. Let  $R_t$  be a random variable corresponding to the number of trials needed in the **repeat** loop from line 4 in FastRegVol at the point when  $|S| = t$ . Note that conditioning on the algorithm's history,  $R_t$  is distributed according to geometric distribution  $\text{Ge}(q_t)$  with success probability:

$$q_t = \frac{1}{t} \sum_{i \in S} (1 - \mathbf{x}_i^\top (\mathbf{X}_S^\top \mathbf{X}_S + \lambda \mathbf{I})^{-1} \mathbf{x}_i) \geq \frac{t-d}{t} \geq \frac{1}{2}.$$

Thus, even though variables  $R_t$  are not themselves independent, they can be upper-bounded by a sequence of independent variables  $\widehat{R}_t \sim \text{Ge}(\frac{t-d}{t})$ . The expectation of the total number of trials in FastRegVol,  $\bar{R} = \sum_t R_t$ , can thus be bounded as follows:

$$\mathbb{E}[\bar{R}] \leq \sum_{t=2d}^n \mathbb{E}[\widehat{R}_t] = \sum_{t=2d}^n \frac{t}{t-d} \leq 2n.$$

Next, we will obtain a similar bound with high probability instead of in expectation. Here, we will have to use the fact that the variables  $\widehat{R}_t$  are independent, which means that we can upper-bound their sum with high probability using standard concentration bounds for geometric distribution. For example, using Corollary 2.2 from Janson (2018) one can immediately show that with probability at least  $1 - \delta$  we have  $\bar{R} = O(n \ln \delta^{-1})$ . However, more careful analysis shows an even better dependence on  $\delta$ .

**Lemma 22** *Let  $\widehat{R}_t \sim \text{Ge}(\frac{t-d}{t})$  be independent random variables. Then, w.p. at least  $1 - \delta$ ,*

$$\sum_{t=2d}^n \widehat{R}_t = O\left(n + \log(n/d) \log(1/\delta)\right).$$

Each trial of rejection sampling requires computing one weight  $h_i$  in time  $O(d^2)$ . The overall time complexity of FastRegVol thus includes computation and updating of matrix  $\mathbf{Z}$  (in time  $O(nd^2)$ ), rejection sampling which takes  $O\left((n + \log(\frac{n}{d}) \log(\frac{1}{\delta})) d^2\right)$  time, and (if  $s < 2d$ ) the RegVol portion, taking  $O(d^3)$ .  $\blacksquare$

**Proof of Lemma 22** As observed by Janson (2018), tail-bounds for the sum of geometric random variables depend on the minimum acceptance probability among those variables. Note that for the vast majority of  $\widehat{R}_t$ 's the acceptance probability is very close to 1, so intuitively we should be able to take advantage of this to improve our tail bounds. To that end, we partition the variables into groups of roughly similar acceptance probability and then separately bound the sum of variables in each group. Let  $J = \log(\frac{n}{d})$  (w.l.o.g. assume that  $J$  is an integer). For  $1 \leq j \leq J$ , let  $I_j = \{d2^j, d2^j + 1, \dots, d2^{j+1}\}$  represent the  $j$ -th partition. We use the following notation for each partition:

$$\bar{R}_j \stackrel{\text{def}}{=} \sum_{t \in I_j} R_t, \quad \mu_j \stackrel{\text{def}}{=} \mathbb{E}[\bar{R}_j], \quad r_j \stackrel{\text{def}}{=} \min_{t \in I_j} \frac{t-d}{t}, \quad \gamma_j \stackrel{\text{def}}{=} \frac{\log(\delta^{-1})}{d2^{j-2}} + 3.$$

Now, we apply Theorem 2.3 of Janson (2018) to  $\bar{R}_j$ , obtaining

$$P(\bar{R}_j \geq \gamma_j \mu_j) \leq \gamma_j^{-1} (1 - r_j)^{(\gamma_j - 1 - \ln \gamma_j) \mu_j} \stackrel{(1)}{\leq} (1 - r_j)^{\gamma_j \mu_j / 4} \stackrel{(2)}{\leq} 2^{-j \gamma_j d 2^{j-2}},$$

where (1) follows since  $\gamma_j \geq 3$ , and (2) holds because  $\mu_j \geq d 2^j$  and  $r_j \geq 1 - 2^{-j}$ . Moreover, for the chosen  $\gamma_j$  we have

$$j \gamma_j d 2^{j-2} = j \log(\delta^{-1}) + 3j d 2^{j-2} \geq \log(\delta^{-1}) + j = \log(2^j \delta^{-1}).$$

Let  $A$  denote the event that  $\bar{R}_j \leq \gamma_j \mu_j$  for all  $j \leq J$ . Applying union bound, we get

$$P(A) \geq 1 - \sum_{j=1}^J P(\bar{R}_j \geq \gamma_j \mu_j) \geq 1 - \sum_{j=1}^J 2^{-\log(2^j \delta^{-1})} = 1 - \sum_{j=1}^J \frac{\delta}{2^j} \geq 1 - \delta.$$

If  $A$  holds, then we obtain the desired bound:

$$\begin{aligned} \sum_{t=2d}^n \hat{R}_t &\leq \sum_{j=1}^J \gamma_j \mu_j \leq \sum_{j=1}^J \left( \frac{\log(\delta^{-1})}{d 2^{j-2}} + 3 \right) d 2^{j+1} = 8J \log(\delta^{-1}) + 6 \sum_{j=1}^J d 2^j \\ &= O\left( \log(n/d) \log(1/\delta) + n \right). \quad \blacksquare \end{aligned}$$

## 6. Experiments

In this section we experimentally evaluate the proposed volume sampling algorithms in terms of runtime and in the task of subsampling for linear regression. We use regularization both for sampling and for prediction, as discussed in Section 4. The list of implemented algorithms is:

- a) Regularized volume sampling (algorithms FastRegVol and RegVol),
- b) Leverage score sampling<sup>13</sup> (LSS) – a popular i.i.d. sampling technique (Mahoney, 2011), where examples are selected w.p.  $P(i) = (\mathbf{x}_i^\top (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{x}_i) / d$ .

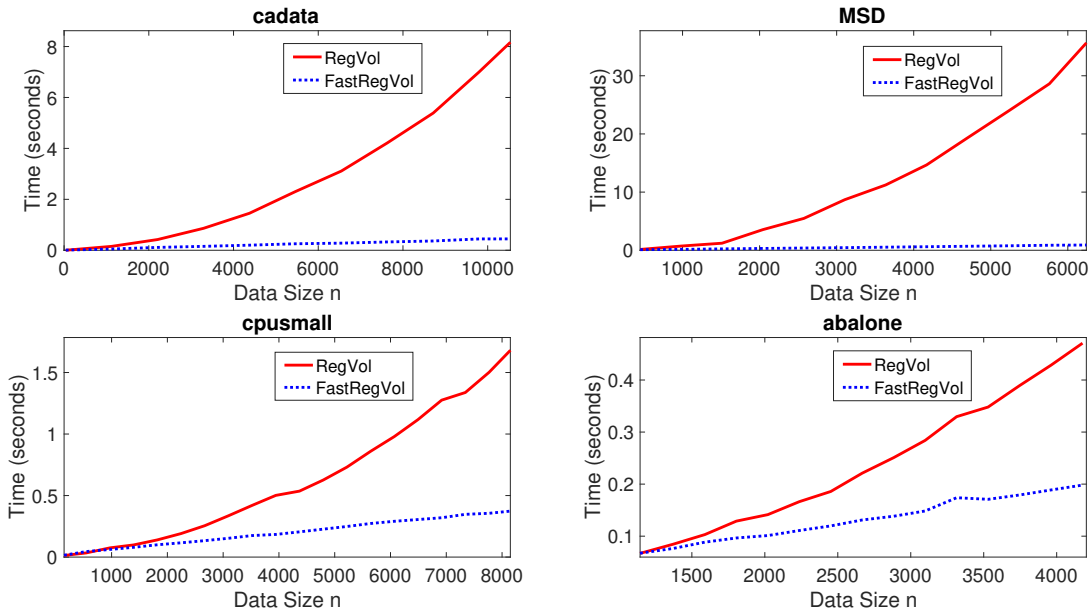
The experiments were performed on several benchmark linear regression datasets from the libsvm repository (Chang and Lin, 2011). Table 1 lists those datasets along with running times for sampling dimension many columns with each method. Dataset MSD was too big for RegVol to finish in reasonable time, however FastRegVol finished in less than 40

Dataset	$n \times d$	RegVol	FastRegVol	LSS
cadata	21k × 8	33.5s	0.9s	0.1s
MSD	464k × 90	>24hr	39s	12s
cpusmall	8k × 12	1.7s	0.4s	0.07s
abalone	4k × 8	0.5s	0.2s	0.03s

seconds. In Figure 6 we plot the runtime against varying values of  $n$  (using portions of the datasets), to compare how FastRegVol and RegVol scale with respect to the data size. We observe that FastRegVol exhibits linear dependence on  $n$ , thus it is much better suited for running on large datasets.

**Table 1:** List of regression datasets with runtime comparison between RegVol and FastRegVol. We also provide the runtime for i.i.d. sampling with exact leverage scores (LSS).

13. Regularized variants of leverage scores have also been considered in context of kernel ridge regression Alaoui and Mahoney (2015). However, in our experiments regularizing leverage scores did not provide any improvements.



**Figure 6:** Comparison of runtime between FastRegVol and RegVol on four libsvm regression datasets (Chang and Lin, 2011), with the methods ran on data subsets of varying size ( $n$ ).

### 6.1 Subset Selection for Ridge Regression

We applied volume sampling to the task of subset selection for linear regression, by evaluating the subsampled ridge estimator  $\mathbf{w}_{\lambda}^*(S)$  using the average loss over the full dataset, i.e.,

$$\text{Average Loss: } \frac{1}{n} \|\mathbf{X} \mathbf{w}_{\lambda}^*(S) - \mathbf{y}\|^2, \quad \text{where } \mathbf{w}_{\lambda}^*(S) = (\mathbf{X}_S^{\top} \mathbf{X}_S + \lambda \mathbf{I})^{-1} \mathbf{X}_S^{\top} \mathbf{y}_S.$$

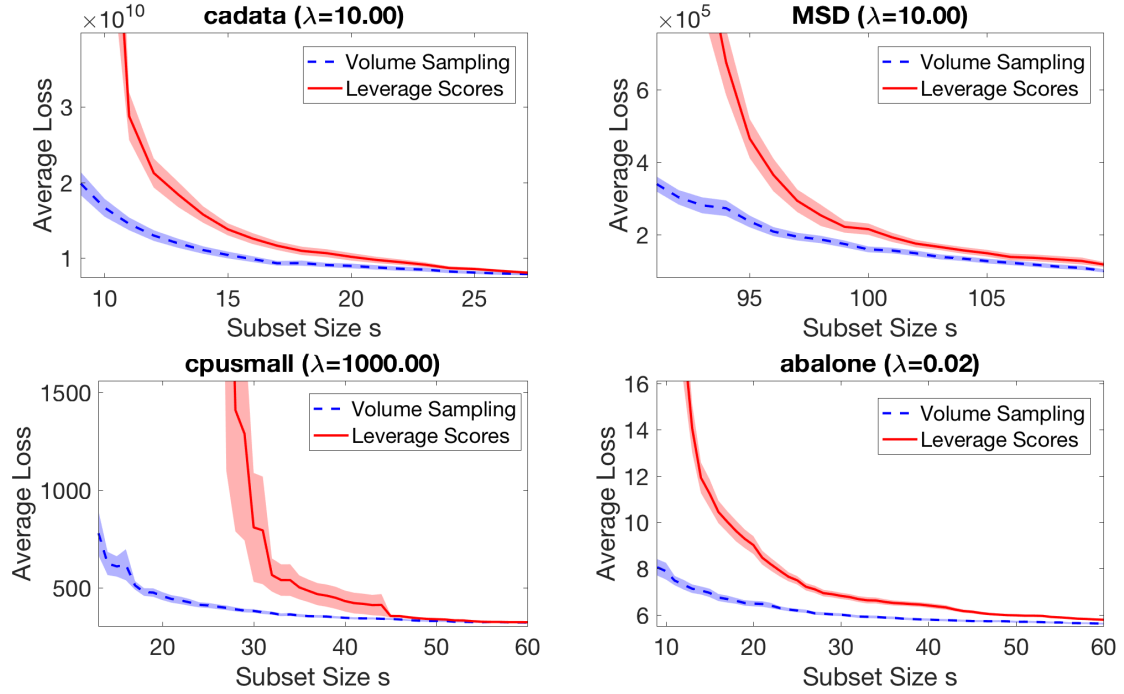
We evaluated the estimators for a range of subset sizes and values of  $\lambda$ , when the subsets are sampled according to  $\lambda$ -regularized volume sampling<sup>14</sup> and leverage score sampling. The results were averaged over 20 runs of each experiment. For clarity, Figure 7 shows the results only with one value of  $\lambda$  for each dataset, chosen so that the subsampled ridge estimator performed best (on average over all samples of preselected size  $s$ ). Note that for leverage scores we did the appropriate rescaling of the instances before solving for  $\mathbf{w}_{\lambda}^*(S)$  for the sampled subproblems (see Mahoney (2011) for details). Volume sampling does not require any rescaling. The results on all datasets show that when only a small number of responses  $s$  is obtainable, then regularized volume sampling offers better estimators than leverage score sampling (as predicted by Theorems 17 and 18). The lower bound from Theorem 18b can be observed for dataset cpusmall, where  $d = 12$  and  $d \log d \approx 30$ .

## 7. Conclusions

Volume sampling is a joint sampling procedure that produces more diverse samples than i.i.d. sampling. We developed a method for proving exact matrix expectation formulas for volume sampling giving further credence to the fact that this is a fundamental sampling procedure. We also made significant progress on finding an efficient implementation of this sampling procedure: Our

14. Our experiments suggest that using the same  $\lambda$  for sampling and for computing the ridge estimator works best.





**Figure 7:** Comparison of loss of the subsampled ridge estimator when using regularized volume sampling vs using leverage score sampling on four datasets.

new reverse iterative volume sampling algorithm runs in time  $O(nd^2)$ . Note that this running time is within a constant factor of i.i.d. sampling with exact leverage scores and is a remarkable feat since volume sampling was only recently shown to be polynomial (that is  $O(n^4s)$  in Li et al. (2017)).

A final long ranging question is how to generalize volume sampling and the exact matrix expectation formulas to higher order tensors.

## Acknowledgments

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## Appendix A. Inductive Proof of Cauchy-Binet

The most common form of the Cauchy-Binet equation deals with two real  $n \times d$  matrices  $\mathbf{A}, \mathbf{B}$ :  $\sum_{S: |S|=d} \det(\mathbf{A}_S^\top \mathbf{B}_S) = \det(\mathbf{A}^\top \mathbf{B})$ . It is easy to generalize volume sampling and Theorem 2 to this “asymmetric” version. Here we give an alternate inductive proof.

For  $i \in \{1..n\}$ , let  $\mathbf{a}_i, \mathbf{b}_i$  denote the  $i$ -th row of  $\mathbf{A}, \mathbf{B}$ , respectively. For  $S \subseteq \{1..n\}$ ,  $\mathbf{A}_S$  consists of all rows indexed by  $S$ , and  $\mathbf{A}_{-i}$ , all except for the  $i$ -th row.

**Theorem 23** For  $\mathbf{A}, \mathbf{B} \in \mathbb{R}^{n \times d}$  and  $n - 1 \geq s \geq d$ :

$$\det(\mathbf{A}^\top \mathbf{B}) = \frac{1}{\binom{n-d}{s-d}} \sum_{S: |S|=s} \det(\mathbf{A}_S^\top \mathbf{B}_S).$$

**Proof**  $S$  is a size  $s$  subset of a set of size  $n$ . We rewrite the range restriction  $n - 1 \geq s \geq d$  for size  $s$  as  $1 \leq n - s \leq n - d$  and induct on  $n - s$ . For the base case,  $n - s = 1$  or  $s = n - 1$ , we need to show that

$$\det(\mathbf{A}^\top \mathbf{B}) = \frac{1}{n - d} \sum_{i=1}^n \det(\mathbf{A}_{-i}^\top \mathbf{B}_{-i}).$$

This clearly holds if  $\det(\mathbf{A}^\top \mathbf{B}) = 0$ . Otherwise, by Sylvester's Theorem

$$\sum_{i=1}^n \frac{\det(\overbrace{\mathbf{A}_{-i}^\top \mathbf{B}_{-i}}^{\mathbf{A}^\top \mathbf{B} - \mathbf{a}_i \mathbf{b}_i^\top})}{\det(\mathbf{A}^\top \mathbf{B})} = \sum_{i=1}^n (1 - \mathbf{a}_i^\top (\mathbf{A}^\top \mathbf{B})^{-1} \mathbf{b}_i) = n - \overbrace{\text{tr}((\mathbf{A}^\top \mathbf{B})^{-1} \mathbf{A}^\top \mathbf{B})}^d.$$

Induction: Assume  $2 \leq n - s \leq n - d$ .

$$\begin{aligned} \det(\mathbf{A}^\top \mathbf{B}) &\stackrel{\text{base case}}{=} \frac{1}{n - d} \sum_{i=1}^n \det(\mathbf{A}_{-i}^\top \mathbf{B}_{-i}) \\ &\stackrel{\text{ind. step}}{=} \frac{1}{n - d} \sum_{i=1}^n \sum_{S: |S|=s, i \notin S} \frac{1}{\binom{n-1-d}{s-d}} \det(\mathbf{A}_S^\top \mathbf{B}_S) \\ &= \underbrace{\frac{n-s}{n-d} \frac{1}{\binom{n-1-d}{s-d}}}_{\frac{1}{\binom{n-d}{s-d}}} \sum_{S: |S|=s} \det(\mathbf{A}_S^\top \mathbf{B}_S). \end{aligned}$$

Note that for the induction step,  $S$  is a subset of size  $s$  from a set of size  $n - 1$  and we have the range restriction  $1 \leq n - 1 - s \leq n - 1 - d$ . Clearly,  $n - 1 - s$  is one smaller than  $n - s$ . For the last equality, notice that each set  $S : |S| = s$  is counted  $n - s$  times in the double sum. ■

## Appendix B. Alternate Proof of Theorem 5

We make use of the following derivative for determinants by Petersen and Pedersen (2012):

$$\text{For symmetric } \mathbf{C}: \quad \frac{\partial \det(\mathbf{X}^\top \mathbf{C} \mathbf{X})}{\partial \mathbf{X}} = 2 \det(\mathbf{X}^\top \mathbf{C} \mathbf{X}) \mathbf{C} \mathbf{X} (\mathbf{X}^\top \mathbf{C} \mathbf{X})^{-1}.$$

The proof begins with generalized Cauchy-Binet for size  $s$  volume sampling:

$$\sum_S \det(\mathbf{X}^\top \mathbf{I}_S \mathbf{X}) = \binom{n-d}{s-d} \det(\mathbf{X}^\top \mathbf{X}).$$

Now, we take a derivative w.r.t.  $\mathbf{X}$  on both sides

$$\begin{aligned} &\sum_S 2 \det(\mathbf{X}^\top \mathbf{I}_S \mathbf{X}) (\mathbf{I}_S \mathbf{X})^{+\top} = \binom{n-d}{s-d} 2 \det(\mathbf{X}^\top \mathbf{X}) \mathbf{X}^{+\top} \\ \Leftrightarrow &\underbrace{\sum_S \frac{\det(\mathbf{X}^\top \mathbf{I}_S \mathbf{X})}{\binom{n-d}{s-d} \det(\mathbf{X}^\top \mathbf{X})} (\mathbf{I}_S \mathbf{X})^{+\top}}_{\mathbb{E}[(\mathbf{I}_S \mathbf{X})^{+\top}]} = \mathbf{X}^{+\top}. \end{aligned}$$

### Appendix C. Proof of Proposition 14

The main idea behind the proof is to construct variants of the input matrix  $\mathbf{X}$  and relate their volumes. We use the following standard properties of the determinant:

**Proposition 24** *For any matrix  $\mathbf{M}$ ,  $\det(\mathbf{M}^\top \mathbf{M}) = \det(\widetilde{\mathbf{M}}^\top \widetilde{\mathbf{M}})$  where  $\widetilde{\mathbf{M}}$  is produced from  $\mathbf{M}$  through the following operations:*

- a)  $\widetilde{\mathbf{M}}$  equals  $\mathbf{M}$  except that column  $\mathbf{m}_j$  is replaced by  $\mathbf{m}_j + \alpha \mathbf{m}_i$ , where  $\mathbf{m}_i$  is another column of  $\mathbf{M}$ ;
- b)  $\widetilde{\mathbf{M}}$  equals  $\mathbf{M}$  except that two rows are swapped.

Recall that our goal is to prove the following formula for any  $\mathbf{X}, \mathbf{y}$  and  $i \in \{1..n\}$ :

$$\det(\mathbf{X}^\top \mathbf{X}) (L(\mathbf{w}^*(-i)) - L(\mathbf{w}^*)) = (\det(\mathbf{X}^\top \mathbf{X}) - \det(\mathbf{X}_{-i}^\top \mathbf{X}_{-i})) \ell_i(\mathbf{w}^*(-i)).$$

By Proposition 24b, we can assume w.l.o.g. that  $i = n$ , i.e. that the test row in Proposition 14 is the last row of  $\mathbf{X}$ . As discussed in Section 3.3, the columns of  $\mathbf{X}$  are the feature vectors, denoted by  $\mathbf{f}_1, \dots, \mathbf{f}_d$ . Moreover, the optimal prediction vector on the full dataset,  $\widehat{\mathbf{y}} = \mathbf{X} \mathbf{w}^*$ , is a projection of  $\mathbf{y}$  onto the subspace spanned by the features/columns of  $\mathbf{X}$ , denoted as  $\widehat{\mathbf{y}} = \mathbf{P}_{\mathbf{X}} \mathbf{y}$ . Let us define a vector  $\bar{\mathbf{y}}$  as

$$\bar{\mathbf{y}}^\top \stackrel{\text{def}}{=} (\text{---} \widehat{\mathbf{y}}_{-n}^\top \text{---}, y_n), \quad (18)$$

where  $\widehat{\mathbf{y}}_{-n} \stackrel{\text{def}}{=} \mathbf{X}_{-n} \mathbf{w}^*(-n)$  is the optimal prediction vector for the training problem  $(\mathbf{X}_{-n}, \mathbf{y}_{-n})$ . Note, that if  $\text{rank}(\mathbf{X}_{-n}) < d$ , then  $\mathbf{w}^*(-n)$  may not be unique, but we can pick any weight vector as long as it minimizes the loss on the training set  $\{1..n-1\}$ . Next, we show the following lemma:

**Lemma 25** *The best achievable loss for the problem  $(\mathbf{X}, \mathbf{y})$  can be decomposed as follows:*

$$L(\mathbf{w}^*) = L(\mathbf{w}^*(-n)) - \ell_n(\mathbf{w}^*(-n)) + \|\bar{\mathbf{y}} - \widehat{\mathbf{y}}\|^2. \quad (19)$$

**Proof** First, we will show that  $\bar{\mathbf{y}}$  is the projection of  $\mathbf{y}$  onto the subspace spanned by all features and the unit vector  $\mathbf{e}_n \in \mathbb{R}^n$  (where  $n$  corresponds to the test row). That is, we want to show that  $\bar{\mathbf{y}} = \mathbf{P}_{(\mathbf{X}, \mathbf{e}_n)} \mathbf{y}$ . Denote  $\tilde{\mathbf{y}}$  as that projection. Observe that  $\tilde{y}_n = y_n$ , because if this was not true, we could construct a vector  $\tilde{\mathbf{y}} + (y_n - \tilde{y}_n) \mathbf{e}_n$  that is closer to  $\mathbf{y}$  than  $\tilde{\mathbf{y}}$  and lies in  $\text{span}(\mathbf{X}, \mathbf{e}_n)$ . Thus, the projection does not incur any loss along the  $n$ -th dimension and can be reduced to the remaining  $n - 1$  dimensions, which corresponds to solving the training problem  $(\mathbf{X}_{-n}, \mathbf{y}_{-n})$ . Using the definition of  $\bar{\mathbf{y}}$  in (18), this shows that  $\tilde{\mathbf{y}} = \mathbf{P}_{(\mathbf{X}, \mathbf{e}_n)} \mathbf{y}$  equals  $\bar{\mathbf{y}}$ .

Next, we will show that  $\widehat{\mathbf{y}}$  is the projection of  $\bar{\mathbf{y}}$  onto  $\text{span}(\mathbf{X})$ , i.e. that  $\mathbf{P}_{\mathbf{X}} \bar{\mathbf{y}} = \widehat{\mathbf{y}}$ . By the linearity of projection, we have

$$\begin{aligned} \mathbf{P}_{\mathbf{X}} \bar{\mathbf{y}} &= \mathbf{P}_{\mathbf{X}}(\bar{\mathbf{y}} - \mathbf{y} + \mathbf{y}) \\ &= \mathbf{P}_{\mathbf{X}}(\bar{\mathbf{y}} - \mathbf{y}) + \mathbf{P}_{\mathbf{X}} \mathbf{y} \\ &= \mathbf{P}_{\mathbf{X}}(\bar{\mathbf{y}} - \mathbf{y}) + \widehat{\mathbf{y}}. \end{aligned}$$

We already showed that  $\bar{\mathbf{y}} = \mathbf{P}_{(\mathbf{X}, \mathbf{e}_n)} \mathbf{y}$ . Therefore, the vector  $\bar{\mathbf{y}} - \mathbf{y}$  is orthogonal to the column vectors of  $\mathbf{X}$ , and thus  $\mathbf{P}_{\mathbf{X}}(\bar{\mathbf{y}} - \mathbf{y}) = 0$ . This shows that  $\mathbf{P}_{\mathbf{X}} \bar{\mathbf{y}} = \widehat{\mathbf{y}}$ .

Finally, note that since  $\bar{\mathbf{y}}$  is the projection of  $\mathbf{y}$  onto  $\text{span}(\mathbf{X}, \mathbf{e}_n)$  and  $\hat{\mathbf{y}} \in \text{span}(\mathbf{X}, \mathbf{e}_n)$ , vector  $\bar{\mathbf{y}} - \mathbf{y}$  is orthogonal to vector  $\bar{\mathbf{y}} - \hat{\mathbf{y}}$  and by the Pythagorean Theorem we have

$$\|\hat{\mathbf{y}} - \mathbf{y}\|^2 = \|\bar{\mathbf{y}} - \mathbf{y}\|^2 + \|\bar{\mathbf{y}} - \hat{\mathbf{y}}\|^2.$$

Using the definition of  $\bar{\mathbf{y}}$  in (18), we have

$$\|\bar{\mathbf{y}} - \mathbf{y}\|^2 = \|\hat{\mathbf{y}}_{-n} - \mathbf{y}_{-n}\|^2 = L(\mathbf{w}^*(-n)) - \ell_n(\mathbf{w}^*(-n)),$$

concluding the proof of the lemma.  $\blacksquare$

**Proof of Proposition 14** We construct a matrix  $\bar{\mathbf{X}}$ , adding vector  $\bar{\mathbf{y}}$  as an extra column to matrix  $\mathbf{X}$ :

$$\bar{\mathbf{X}} \stackrel{\text{def}}{=} (\mathbf{X}, \bar{\mathbf{y}}) = \left( \begin{array}{c|c} \mathbf{X}_{-n} & \hat{\mathbf{y}}_{-n} \\ \hline \mathbf{x}_n^\top & y_n \end{array} \right). \quad (20)$$

Applying “base  $\times$  height” and Lemma 25, we compute the volume spanned by  $\bar{\mathbf{X}}$ :

$$\det(\bar{\mathbf{X}}^\top \bar{\mathbf{X}}) = \det(\mathbf{X}^\top \mathbf{X}) \|\bar{\mathbf{y}} - \hat{\mathbf{y}}\|^2 = \det(\mathbf{X}^\top \mathbf{X}) (L(\mathbf{w}^*) - L(\mathbf{w}^*(-n)) + \ell_n(\mathbf{w}^*(-n))). \quad (21)$$

Next, we use the fact that volume is preserved under elementary column operations (Proposition 24a). Note, that prediction vector  $\hat{\mathbf{y}}_{-n}$  is a linear combination of the columns of  $\mathbf{X}_{-n}$ , with the coefficients given by  $\mathbf{w}^*(-n)$ . Therefore, looking at the block structure of  $\bar{\mathbf{X}}$  (see (20)), we observe that performing column operations on the last column of  $\bar{\mathbf{X}}$  with coefficients given by negative  $\mathbf{w}^*(-n)$ , we can zero out that column except for its last element:

$$\bar{\mathbf{y}} - \mathbf{X} \mathbf{w}^*(-n) = r \mathbf{e}_n,$$

where  $r \stackrel{\text{def}}{=} y_n - \mathbf{x}_n^\top \mathbf{w}^*(-n)$  (see transformation (a) in (22)). Now, we consider two cases, depending on whether or not  $r$  equals zero. If  $r \neq 0$ , then we further transform the matrix by a second transformation (b), which zeros out the last row (the test row) using column operations. The entire sequence of operations, resulting in a matrix we call  $\bar{\mathbf{X}}_0$ , is shown below:

$$\bar{\mathbf{X}} = \left( \begin{array}{c|c} \mathbf{X}_{-n} & \hat{\mathbf{y}}_{-n} \\ \hline \mathbf{x}_n^\top & y_n \end{array} \right) \xrightarrow{\text{(a)}} \left( \begin{array}{c|c} \mathbf{X}_{-n} & 0 \\ \hline \mathbf{x}_n^\top & r \end{array} \right) \xrightarrow{\text{(b)}} \left( \begin{array}{c|c} \mathbf{X}_{-n} & 0 \\ \hline 0 & r \end{array} \right) = \bar{\mathbf{X}}_0. \quad (22)$$

Note, that due to the block-diagonal structure of  $\bar{\mathbf{X}}_0$ , its volume can be easily described by the “base  $\times$  height” formula:

$$\det(\bar{\mathbf{X}}_0^\top \bar{\mathbf{X}}_0) = \det(\mathbf{X}_{-n}^\top \mathbf{X}_{-n}) r^2 = \det(\mathbf{X}_{-n}^\top \mathbf{X}_{-n}) \ell_n(\mathbf{w}^*(-n)). \quad (23)$$

Since  $\det(\bar{\mathbf{X}}^\top \bar{\mathbf{X}}) = \det(\bar{\mathbf{X}}_0^\top \bar{\mathbf{X}}_0)$ , we can combine (21) and (23) to obtain the desired result.

Finally, if  $r = 0$  we cannot perform transformation (b). However, in this case matrix  $\bar{\mathbf{X}}$  has volume 0, and moreover,  $\ell_n(\mathbf{w}^*(-n)) = r^2 = 0$ , so once again we have

$$\det(\bar{\mathbf{X}}^\top \bar{\mathbf{X}}) = 0 = \det(\mathbf{X}_{-n}^\top \mathbf{X}_{-n}) \ell_n(\mathbf{w}^*(-n)),$$

which concludes the proof of Proposition 14.  $\blacksquare$

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