How bad is worst-case data if you know where it comes from?*

Justin Y. Chen
gvaliant@cs.stanford.edu

Gregory Valiant
pvaliant@gmail.com

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Abstract

We introduce a framework for studying how distributional assumptions on the process by which data is partitioned into a training and a test set can be leveraged to provide accurate estimation or learning algorithms, even for worst-case datasets. Specifically, we consider a setting of \( n \) datapoints, \( x_1, \ldots, x_n \), together with a specified distribution, \( P \), over partitions of these datapoints into a training set, test set, and irrelevant set. An algorithm takes as input a description of \( P \) (or sample access to \( P \)), the indices of the test and training sets, and the datapoints in the training set, and it returns a model or estimate that will be evaluated on the datapoints in the test set. We evaluate an algorithm in terms of its worst-case expected performance: the expected performance over potential test/training sets, for worst-case datapoints, \( x_1, \ldots, x_n \).

For what distributions, \( P \), over test/training splits, and what estimation or learning tasks, is it possible to achieve good worst-case expected performance? How do optimal algorithms leverage the distribution, \( P \)? This framework is a significant departure from the more typical distributional assumptions on the datapoints (e.g. that data is drawn independently, or according to an exchangeable process from some distribution), and can model a number of natural data collection processes, including processes where certain individuals/datapoints have an affinity to be included in the test set but not the training set, processes with dependencies such as “snowball sampling” and “chain sampling” where membership in test and training sets is governed by stochastic processes (e.g. over social networks), and settings where test and training sets satisfy chronological constraints (e.g. the test instances were observed after the training instances). Crucially, this framework considers worst-case data, and hence makes no assumptions about the underlying datapoints.

Within this framework, we consider the setting where the datapoints \( \{x_1, \ldots, x_n\} \) are bounded real numbers, and the goal is to estimate the mean of the test set. We give an efficient algorithm that returns a weighted combination of the training set—whose weights depend on the distribution, \( P \), and on the training and test set indices—and show that the worst-case expected error achieved by this algorithm is at most a multiplicative \( \pi/2 \) factor worse than the optimal of such algorithms. The algorithm, and its proof, leverage a surprising connection to the Grothendieck problem.

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1 Modeling Data Collection

For many real-world learning or prediction problems, it is not unreasonable to assume that data is drawn independently from some underlying distribution; correspondingly, there is an enormous body of work developing algorithms suited for such settings, or for related settings satisfying slightly weaker assumptions such as exchangeability. There are also many settings in which we know very little about the underlying data, and any sort of distributional assumption would be problematic. For such settings, however, we might have some knowledge or control over the process by which data is collected to form a training set, and the process that generates the test set on which we will make predictions or deploy our trained model. How can we design learning algorithms that are optimal for a given data collection process? For which data collection processes is accurate estimation or learning possible, even for worst-case data? Surprisingly, there seems to be little work on such questions.

Here, we introduce a general framework in which to study these questions. Consider a set of potential datapoints, \( X = \{x_1, \ldots, x_n\} \) and a distribution, \( P \), over partitions of \( X \) into a test set, training set, and irrelevant set. A learning algorithm will receive as input a description of \( P \) (or sample access), the identities of the datapoints in the training set along with their values, and the identities of the elements in the test set, and returns a model whose performance will be evaluated on the datapoints in the test set. We neither observe, nor are evaluated on the datapoints in the irrelevant set. The worst-case expected performance of the algorithm can now be defined as the expected performance of the algorithm over worst-case datasets, \( X \), where the expectation is with respect to \( P \)—the joint distribution modeling the process of how the training and test sets are formed. The following example illustrates the components of this formulation.

**Example 1.** Suppose there are \( n = 10 \) people in our office, \{Alice, Bob, Carol, \ldots, Yolanda\}, and a joint distribution \( P \) modeling membership in a training and test set, e.g. Alice is in the training, test, or irrelevant set independently with probability \( 1/3 \), Bob’s membership is positively correlated with Alice’s, etc. The goal is to return an estimate of the mean salary of the people in the test set, given the salaries and names of Alice, Carol, and Fred, and are asked to estimate the mean income of Yolanda and Charles. Our goal is to design an estimator that leverages its knowledge of the joint training/test distribution \( P \) in an optimal way, in expectation over the randomness of which test/training sets are selected, in a worst-case sense over the underlying values of the datapoints (i.e. adversarially chosen salaries).

Ultimately, one might hope to analyze a hybrid model that leverages both distributional assumptions about the datapoints, as well as knowledge about the training/test set generation. In this paper, we focus on the scenario where all of our knowledge is about the training/test set generation and we have no assumptions about the data; considering this extreme setting is one natural starting place from which to explore the role of this new type of assumption.

For the purpose of this paper, we will focus on the most basic setting of our framework where each datapoint, \( x_i \), is a real number in the interval \([-1, 1]\), and the goal is to estimate the mean of the test set. Understanding which joint distributions \( P \) admit algorithms with subconstant worst-case expected estimation error is a fundamental question for this framework. Additionally, the ability to accurately estimate the mean of the test set can be used in a black-box fashion to estimate a number of other useful quantities, enabling applications such as performing linear regression. We briefly discuss such extensions to more complex learning settings in Section 1.3.
To motivate this framework and provide some intuition for how existing results can be expressed in this model, we begin with some illustrative examples:

**Example 2 (Independent Partitions).** Consider the setting where the joint training/test distribution \( P \) corresponds to assigning each datapoint \( x_i \in \{ x_1, \ldots, x_n \} \) independently to either the test or training set, with probability 1/2. In this setting, the test and training set means both concentrate around \( \frac{1}{n} \sum x_i \)—the mean across all items in the universe—and hence even for worst-case datasets, the algorithm that simply returns the training set mean will have expected squared error \( O(1/n) \).

A slight variant of this setting could have \( P \) defined via two sets of \( n \) probabilities, \( p_1, \ldots, p_n \) and \( q_1, \ldots, q_n \), where each datapoint \( x_i \) is independently in the test set with probability \( p_i \), training set with probability \( q_i \), irrelevant set with probability \( 1 - p_i - q_i \). In this case, provided the \( p_i \)'s and \( q_i \)'s are bounded away from 0, the test and training means are still concentrated (possibly around different values), and accurate estimation is still possible with expected squared error \( O(1/n) \) via “importance sampling”.

The above example illustrates one way in which accurate estimation is possible, even for worst-case data: namely if both the test and training means are concentrated. The following example illustrates the intuition that if the test and training sets are completely disjoint, then accurate estimation is impossible.

**Example 3.** Suppose every training set in the support of \( P \) is a subset of \( \{ x_1, \ldots, x_{n/2} \} \), and every test set is a subset of \( \{ x_{n/2+1}, \ldots, x_n \} \). In this case, it is impossible to estimate the test mean with worst-case error less than 1. To see this, consider the assignment to datapoints where \( x_1, \ldots, x_{n/2} = 0 \), and where either \( x_{n/2+1} = \ldots = x_n = 1 \) or \( x_{n/2+1} = \ldots = x_n = -1 \) independently with probability 1/2. No algorithm can distinguish these cases based on the training set, and hence the worst-case expected error is 1, achieved by the trivial algorithm that always guesses 0.

The following example illustrates that accurate prediction can still be possible, even for a distribution for which the test (and training) means have constant variance across possible choices of the test and training set. This example captures a setting where the distribution, \( P \), respects chronological constraints, in the sense that, for any test/training set that has non-zero probability under \( P \), if \( x_i \) is in the test set and \( x_j \) is in the training set, \( j < i \). Such constraints mirror the many settings where the training set corresponds to past data, and the test set corresponds to data that will be received in the future. Here, treating data as being worst-case corresponds to not making any assumptions that the world is “stationary”—future datapoints might not be like past datapoints.

**Example 4 (“Selective” Prediction).** Consider the joint training/test distribution \( P \) corresponding to the following process: a time \( t \) is drawn uniformly from \( \{ 1, \ldots, n - 1 \} \), and the training set is \( \{ x_1, \ldots, x_t \} \). Then \( w \) is drawn uniformly from \( \{ 1, 2, 4, 8, \ldots, 2^{\log n - 1} \} \) and the test set is \( \{ x_{t+1}, \ldots, x_{\min(x+w,n)} \} \), with the remaining \( x_i \)'s in the irrelevant set. (This prediction task corresponds to choosing a day at random, and deciding to make a prediction about the average change in the stock market over the next \( w \) days.) In this setting, the main results in [2][17] imply that there exists an algorithm whose worst-case expected squared error is \( O(1/\log n) \), and that this is optimal to constant factors. The prediction algorithm achieving this performance is extremely simple: when asked to predict the mean of the next \( w \) data items after \( t \), return the mean of the most recent \( w \) training points, \( \frac{1}{w} \sum_{i=t-w+1}^t x_i \). The results of [17] further imply that this error is the best that can be achieved for any distribution, \( P \), that (1) respects the chronological constraint that training points

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must have lower indices than test points and (2) respects the constraint that test points must form a contiguous block of indices. The surprising aspect of this example is that subconstant expected accuracy is achievable, despite there being no distributional assumptions on the $x_i$s and hence no guarantees that future datapoints are like past datapoints. The randomness in both $t$ and in the window length $w$ of the test set (which define the distribution $P$) are both essential for achieving subconstant worst-case expected accuracy: if $w$ is any fixed value, then the worst-case estimation error is constant.

A fourth example that fits cleanly within our framework is the class of data collection schemes referred to as snowball sampling or chain sampling [9]. In such a scheme, people who have contributed data are asked (or often incentivized) to recruit their acquaintances to contribute data, and the pool of respondents grows, like a snowball. These schemes are frequently used to collect data from sensitive populations, such as drug users. Our framework provides a natural way to model such a sampling process:

**Example 5 (Snowball Sampling).** Suppose datapoints $x_1, \ldots, x_n$ are located at nodes of a social network. A training set is drawn by independently selecting one (or several) indices and then, each index in the training set “recruits” each of its friends in the social network (say independently with probability $p$). The training set will then correspond to the indices that have been recruited in the first $t$ iterations of this “viral” process. The test set could correspond to those nodes recruited in iterations $t+1, \ldots, t+w$ for some horizon $w$, or the test set could be drawn according to an independent snowball sampling process. How do structural properties of the underlying social network translate into positive or negative results on the worst-case expected performance of an optimal estimation algorithm? And how does such an optimal estimation algorithm leverage knowledge of the network structure? While we do not have simple rules-of-thumb for these questions, our main results can certainly be applied to arbitrary settings of such data collection processes.

### 1.1 Summary of Results

Our results focus on linear schemes, which we define to mean that the returned estimate is a linear combination of the training datapoints, where the weights can be an arbitrary function of the test and training indices (but cannot depend on the values of the training datapoints).

**Definition 1.** A linear estimation algorithm, $L$, is a mapping from a set of training indices $A = (a_1, \ldots, a_{|A|}) \subset \{1, \ldots, n\}$ and set of test indices $B = (b_1, \ldots, b_{|B|}) \subset \{1, \ldots, n\}$ to a list of $|A|$ weights, $w_1, \ldots, w_{|A|}$ that may depend on $A$ and $B$. The estimate produced by algorithm $L$ when given the training data corresponding to $A$, $(x_{a_1}, \ldots, x_{a_{|A|}})$ and test indices $B$, is $\sum_{i=1}^{|A|} w_i x_{a_i}$.

Although the class of linear algorithms is restrictive, nearly all natural estimation algorithms that we are aware of fall into this class. The optimal algorithms of Examples 2 and 4, for example, are linear schemes. In the case of the selective predictions setting of Example 4, the constant-factor optimal scheme is linear and the weights depend on the set of test indices, not just on the training indices (recall that the returned estimate is the average of the $w$ highest-indexed training points, where $w$ is the size of the test set). Studying this class of linear algorithm also seems like a natural starting place for considering the general framework.

Although we focus on linear schemes, the example below illustrates the existence of instances where there is a gap between the worst-case expected error of the optimal linear scheme, and the
worst-case expected error of an optimal (nonlinear) scheme. As we discuss in Section 1.3, one of the main open questions is to understand the severity of this gap between linear, and arbitrary algorithms.

Example 6. Let \( n = 4 \). Consider the distribution over partitions of the data indices \( \{1, 2, 3, 4\} \) that assigns a 0.3 probability to the following pairs of training/test indices \( \{(1, 3), (2, 4)\}, \{(2, 4), (1, 3)\}, \{(3, 4), (1, 2)\} \) and a 0.05 probability to \( \{(1, 3), (2)\} \) and \( \{(2, 3, 4), (1)\} \). The optimal linear scheme achieves worst-case expected squared error 0.6652, compared to 0.6627 for the optimal nonlinear scheme. Hence even for training/test set distributions over \( n = 4 \) datapoints, linear schemes are not always worst-case optimal.

A second observation, illustrating a counterintuitive aspect even of linear algorithms, is that there exist joint training/test distributions \( P \) such that the optimal linear scheme assigns negative weights to some training points:

Example 7. Let \( n = 3 \). Consider the distribution over partitions of the data indices \( \{1, 2, 3\} \) that assigns a 1/3 probability to each of the following pairs of training/test indices \( \{(1), (2, 3)\}, \{(2), (1, 3)\}, \{(1, 3), (2)\} \). In the worst-case optimal linear scheme, when the training set contains only \( x_1 \), the corresponding weight is 0.399. When the training set contains only \( x_2 \), the weight is 0.024. And, when the training set contains points \( x_1 \) and \( x_3 \), the respective weights are -0.212 and 0.238. The intuitive explanation for the negative weight is as follows: when the training set contains only \( x_1 \) or only \( x_2 \), the positive weights produce more accurate estimates if \( x_1 \) and \( x_2 \) are similar, and hence a worst-case dataset would want \( x_1 \) and \( x_2 \) to be dissimilar. Putting a negative weight on \( x_1 \) in the case where our training set contains both \( x_1 \) and \( x_3 \) hedges against such datasets, improving the worst-case expected performance. Since we are considering the expected error across the potential training/test splits for worst-case underlying data, the choice of weights on any given training set will depend on the weights used for other training sets, leading to counterintuitive phenomena like negative weights.

Our main result is that there exists an efficient algorithm which, given sample-access to the joint training/test distribution \( P \), returns a linear estimation scheme whose performance is within a constant factor of the worst-case optimal linear scheme for \( P \).

Theorem 1. Let \( P \) denote a distribution over partitions of \( \{1, \ldots, n\} \) into sets \( A, B, \) and \( C \), and let \( \epsilon > 0 \) be a fixed error parameter. There is an algorithm \( L \) which, given sample-access to \( P \) and given sets \( A = (\alpha_1, \ldots, \alpha_{|A|}) \) and \( B = (\beta_1, \ldots, \beta_{|B|}) \), takes poly(n,1/\epsilon) samples from \( P \), runs in time poly(n,1/\epsilon), and returns a list of \( |A| \) weights, \( w_1^{L(A,B)}, \ldots, w_{|A|}^{L(A,B)} \), with the following guarantee: for any dataset \( (x_1, \ldots, x_n) \) with \( |x_i| \leq 1 \), for \( A, B \) drawn from \( P \), with high probability over \( L \)'s samples from \( P \), the expected squared difference between the estimate \( \sum_{i=1}^{|A|} w_i^{L(A,B)} x_{\alpha_i} \) and the test set mean \( \frac{1}{|B|} \sum_{i=1}^{|B|} x_{\beta_i} \), is within an additive \( \epsilon \) and multiplicative \( \pi/2 \) factor of the lowest possible worst-case expected error of any linear scheme. Formally,

\[
\mathbb{E}_{(A,B) \sim P} \left[ \left( \sum_{i=1}^{|A|} w_i^{L(A,B)} x_{\alpha_i} - \frac{1}{|B|} \sum_{i=1}^{|B|} x_{\beta_i} \right)^2 \right] 
\leq \epsilon + \frac{\pi}{2} \left( \inf_{L^*: (A,B) \to \{w_i^{L^*(A,B)}\}} \sup_{(x_1, \ldots, x_n): |x_i| \leq 1} \mathbb{E}_{(A,B) \sim P} \left[ \left( \sum_{i=1}^{|A|} w_i^{L^*(A,B)} x_{\alpha_i} - \frac{1}{|B|} \sum_{i=1}^{|B|} x_{\beta_i} \right)^2 \right] \right). 
\]
The ratio $\frac{\pi}{2}$ to which we approximate the performance of the best linear algorithm is motivated by the fact that, even for a fixed linear algorithm, estimating its worst-case expected performance to within a $\frac{\pi}{2}$ factor is NP-hard. We discuss this in Section 2.2.

1.2 Related Work

There has been a significant recent effort to develop algorithms for estimation and learning that have strong performance guarantees beyond the idealized setting where data is independently drawn from some fixed distribution. This includes the recent body of work on robust learning and statistics. Building off a long line of work from the Statistics community (see e.g. [11, 20]), the models considered in these works assume that datapoints are drawn independently from some distribution of interest, and then an $\alpha$ fraction of datapoints are corrupted arbitrarily/adversarially. (Some of these works also consider the slightly weaker contamination model where the $\alpha$ fraction of arbitrary data is specified before the $1 - \alpha$ fraction of i.i.d. data is drawn.) Recent work from the TCS community developed computationally efficient algorithms for basic estimation and learning tasks in these settings, beginning with estimating the mean and covariance of a high-dimensional Gaussian [6, 15], and subsequently considering more general optimization problems over data, including linear regression [2, 19, 14, 12]. While this work relaxes the typical assumption that all datapoints are drawn i.i.d. from a distribution, the results all crucially leverage the assumption that a significant fraction of the data is still drawn from a well-behaved distribution. From a technical perspective, these works can be viewed as analyzing the structure of the $1 - \alpha$ fraction of i.i.d. datapoints, and then arguing that the adversarial datapoints cannot completely obscure this structure. In this sense, the distributional assumptions on the $1 - \alpha$ fraction of “good” data are critically leveraged.

There is also a line of recent work developing algorithms that work on truncated data [4, 5] which captures one commonly arising class of dataset that deviates from the i.i.d. setting. Here, the assumption is that data is drawn independently from a “nice” distribution—a high-dimensional Gaussian in the case of [4]—but then the dataset is truncated, revealing only the portion that lies within some specified set. The challenge is that this conditioning often significantly skews the statistics of the data. Work on learning from truncated samples differs significantly from the framework considered in our paper, in that the positive results in [4, 5] leverage assumed structure of the underlying data: the Gaussian assumption in [4], and the assumptions of an underlying noisy linear model and that the truncation procedure is only a function of the label of each datapoint, in [5].

Beyond the dependencies that truncation introduces, recent work also considers regression in a setting with more complex dependencies, that models the type of dependence that may arise when datapoints correspond to nodes within a network [3]. In that work, the authors revisit the standard noisy linear regression model where each label $y_i = \theta^T x_i + \epsilon_i$, and the standard logistic regression model where $Pr[y_i = 1] = 1/(1 + exp(\theta^T x_i))$. Instead of assuming that the $\epsilon_i$ and logistic outcomes are drawn independently, they consider the case where these are generated in a correlated fashion, corresponding to a known/fixed covariance matrix with an unknown strength parameter. Despite these dependencies, the authors provide an efficient algorithm for learning the model, $\theta$, in this setting, that still achieves the error guarantees of the independent settings, provided some mild assumptions are satisfied.

Finally, it is worth clarifying the distinction between our framework, and the on-line learning and agnostic learning frameworks. As with our framework, much of the work in on-line learning
makes no assumptions about the underlying data, and often even assumes that the underlying data
is adaptively responding to our predictions. Beyond this, the frameworks are quite different: our
framework considers the task of making a single prediction, as opposed to a sequence of predictions.
Additionally, we are measuring the performance of algorithms in terms of their expected error (or
expected squared error), not in comparison to some set of fixed benchmarks. The agnostic learning
framework is also significantly different from our setting, as it posits access to independent draws
from some (possibly unknown) distribution of examples, and the goal is to return a hypothesis that
accurately reflects whatever structure is present in this distribution. By contrast, in our framework
there is no distribution (or notion of “true structure”) underlying the datapoints, and instead our
distributional assumptions model only the connection between the indices of the test and training
set.

1.3 Discussion and Open Directions

This work introduces a framework for understanding estimation and learning in settings where we
make no assumptions on the datapoints themselves, but can accurately model the process by which
training and evaluation datasets are collected. We hope that further work in this framework will
serve as an enlightening counterpoint to the large body of work that makes strong distributional
assumptions on the data. Below, we outline several open questions, some concrete and some more
conceptual.

Beyond Linear Algorithms: Our main result is an efficient algorithm which, given sample-
access to the distribution $P$ over test/train partitions, the training set, and the set of test indices,
returns a linear estimate of the test set mean, whose expected error (for worst-case data) is within
a multiplicative constant factor of the optimal linear scheme. Example 6 illustrates that linear
schemes are not always optimal. Perhaps the most pressing concrete open question is to bound the
size of this gap between linear and non-linear schemes:

**Question 1.** For every distribution over partitions, $P$, is there a linear algorithm (see Definition 1)
whose worst-case expected error is within a constant factor of the optimal (non-linear) scheme? If
not, how does this gap scale with the number of datapoints, $n$?

If there is a significant gap between linear and non-linear schemes, the natural next question
would be to develop near-optimal non-linear algorithms. Naively, even if we restrict the data to
take values in $\{-1, 1\}$, non-linear algorithms have $O(2^n \cdot \text{support}(P))$ possible parameters while
linear algorithms have $O(n \cdot \text{support}(P))$ possible parameters.

Beyond Mean Estimation: In this work, we focus on estimating the arithmetic mean of the
datapoints in the test set. Our results trivially yield algorithms for estimating certain other func-
tionals of the test set, such as the variance, and higher moments. One can also consider a number
of natural learning tasks within our framework of worst-case data with a known distribution over
partitions into test/training sets. For example, consider a potential dataset $(x_1, y_1), \ldots, (x_n, y_n)$ of
pairs of labeled data, with $x_i \in \mathbb{R}^d$ and the label $y_i \in \mathbb{R}$. Given a distribution, $P$, over partitions
of $\{1, \ldots, n\}$ into a test set, training set, and irrelevant set, as above we can consider an algorithm
which takes as input sample access to $P$, a set of training indices, $A$, and training datapoints,
$(x_A, y_A)$, and set of test indices $B$, and returns a model $f_{P, A, B, (x_A, y_A)}: \mathbb{R}^d \to \mathbb{R}$ that will be applied
to the test points.
One natural measure of performance is the difference between the prediction error of the returned model on the test set, and (for example), the smallest error that any linear model can achieve on this specific test set. The overall goal would then be to minimize the expectation of this difference, over worst-case datasets:

\[
sup_{(x_1,y_1),\ldots,(x_n,y_n)} \left( \mathbb{E}_{(A,B)\sim P} \left[ \sum_{i\in B} (f_{P,A,B}(x_A) - y_i)^2 \right] - \mathbb{E}_{(A,B)\sim P} \left[ \inf_{\theta \in \mathbb{R}^d} \left( \sum_{i\in B} (\theta^T x_i - y_i)^2 \right) \right] \right).
\]

This is quite different (and more challenging) than comparing against the performance of the best linear model over the entire set of \(n\) datapoints; specifically, the model we are being compared against is allowed to vary arbitrarily from test set to test set (the optimization over \(\theta\) is inside the expectation).

Results on mean estimation trivially translate to results in this prediction setting, provided we measure performance against the optimal linear model, \(\theta\), of bounded norm. This follows from observing that the calculation of the optimal linear model on the test set can be viewed as estimating the mean of each of \(O(d^2)\) univariate quantities, including, e.g., the entries of the \(d \times d\) data covariance matrix. A natural question is the extent to which one can improve upon the implications provided by such black-box applications of mean estimation.

**Necessary and Sufficient Conditions for Subconstant Estimation Error:** Our main result can be viewed as a characterization of which joint training/test distributions \(P\) admit linear estimation schemes achieving good worst-case expected error. Still, it would be helpful to extract some high-level interpretable properties of \(P\) that imply, say, the possibility of subconstant (or inverse polynomial) error, or properties that imply that the worst-case expected error will be constant for any algorithm. For the many settings where we have control over how data is collected, such properties could serve to guide the design of these data collection pipelines. Additionally, there might be significant value in articulating sufficient conditions under which simple algorithms—algorithms that are significantly simpler than our convex optimization approach—achieve good worst-case error.

To this end, there are a number of natural conditions that ensure that the test and training sets have sufficient randomness to guarantee that the test and training set means concentrate, such as bounded pairwise dependencies of membership of datapoints in the test set (or training set). Such conditions, however, might be less exciting than the positive results of instances such as Example \(\#1\) where accurate estimation is possible despite test and training means not concentrating. For such instances, any algorithm with subconstant error will need to directly tease apart how the test and training sets are related via \(P\).

Finally, it also seems worthwhile considering this framework from the perspective of specific classes of distribution. For example, for \(P\) corresponding to snowball-sampling over a social network, what network properties imply subconstant estimation error? Are there subtle variants of snowball-sampling that yield significantly better or worse values of the expected estimation error for worst-case data?

### 2 Connections to the Grothendieck Problem

In this section, we establish the connection between the worst-case performance of a given linear estimation algorithm, and the Grothendieck problem. We begin by establishing the notation that...
will be used throughout the remainder of the paper.

2.1 Notation and Preliminaries

Given data $x_1, \ldots, x_n$ from which both the training and test sets are drawn, the main component of our model is a joint distribution on the training and test sets, which are both subsets of $\{1, \ldots, n\}$. Letting $A$ denote the indices in $\{1, \ldots, n\}$ of the training set, and letting $B$ denote the indices of the test set, we allow for an arbitrary joint sampling process $(A, B) \leftarrow \{1, \ldots, n\}$, over pairs of subsets of $\{1, \ldots, n\}$. Such a joint distribution can be approximated to arbitrary accuracy as an unweighted distribution over a list $P$ of pairs $(A_i, B_i)$, and for ease of notation, we adopt this representation here.

**Definition 2.** A joint training/test distribution over a universe of $n$ items is specified by a list $P$ of pairs $(A_i, B_i)$ of some length $m$, where for each $i \in \{1, \ldots, m\}$ the sets $A_i, B_i$ are subsets of $\{1, \ldots, n\}$. To sample from this distribution, choose a uniformly random $i \leftarrow \{1, \ldots, m\}$ and let $A_i$ be the identities of the training set elements, and $B_i$ be the identities of the test set elements. For data $x_1, \ldots, x_n$, the training set will be $x_{A_i}$ and the test set will be $x_{B_i}$.

Given a sampled training set $A$ and test set $B$ from such a distribution, and given a universe of underlying data $x_1, \ldots, x_n$, the algorithmic challenge is to predict a desired attribute of the set of test data $x_B$, given the set of training data $x_A$ along with the identities of $A$ and $B$. Throughout, we focus on the case where the datapoints are real numbers, of magnitude at most 1, and the goal is to compute the arithmetic mean of the test data.

**Definition 3.** For an estimation algorithm $f(x_A, A, B)$ taking as inputs the training data along with the identities of the training set and test set, define its performance, for fixed data $x_1, \ldots, x_n$ on a test/training distribution $P$ to be the mean squared error of its estimation:

$$\frac{1}{m} \sum_{i=1}^{m} (f(x_A, A_i, B_i) - \text{mean}(x_{B_i}))^2$$

When the data $x_1, \ldots, x_n$ are not specified, we characterize an algorithm $f$ by its worst-case performance

$$\max_{x_1, \ldots, x_n \in [-1, 1]} \frac{1}{m} \sum_{i=1}^{m} (f(x_A, A_i, B_i) - \text{mean}(x_{B_i}))^2$$

A crucial special case is linear algorithms, where it will be convenient to introduce further notation.

**Definition 4.** Given a training/test distribution $P = (A_1, B_1), \ldots, (A_m, B_m)$, define for each $B_i$ a corresponding vector $b_i \in \mathbb{R}^n$ where $b_i(j) = \frac{1}{|B_i|}$ for $j \in B_i$ and 0 otherwise. Thus for a vector $x \in \mathbb{R}^n$, we may represent the mean as a vector-vector product, $\text{mean}(x_{B_i}) = b_i^T x$.

**Definition 5.** Given a training/test distribution $P = (A_1, B_1), \ldots, (A_m, B_m)$, a linear estimation algorithm consists of a vector $a_i \in \mathbb{R}^n$ for each $i \in \{1, \ldots, m\}$, where the support of $a_i$ is a subset of $A_i$. Thus the estimate $f(x_{A_i}, A_i, B_i)$ is simply evaluated as the vector-vector product $a_i^T x$. 

\[8\]
Combining the previous two definitions yields that the performance of a linear estimation algorithm \((a_i)\) equals

\[
\max_{x_1, \ldots, x_n \in \{-1, 1\}} \frac{1}{m} \sum_{i=1}^{m} ((a_i - b_i)^T x)^2 = \max_{x_1, \ldots, x_n \in \{-1, 1\}} x^T \left( \frac{1}{m} \sum_{i=1}^{m} (a_i - b_i)^T (a_i - b_i) \right) x \tag{1}
\]

In the second expression above, we (equivalently) restrict the range of each \(x_j\) to the endpoints \([-1, 1]\) since the expression being maximized is a positive semidefinite quadratic form of \(x\), and thus each \(x_j\) may be moved to one of the endpoints of its range without decreasing the objective function.

**Definition 6.** Given a training/test distribution \(P = (A_1, B_1), \ldots, (A_m, B_m)\), the performance of the best linear algorithm is

\[
\frac{1}{m} \min_{a_i: \{j: a_i(j) \neq 0\} \subseteq A_i} \max_{x_1, \ldots, x_n \in \{-1, 1\}} \sum_{i=1}^{m} ((a_i - b_i)^T x)^2
\]

### 2.2 Worst-Case Performance of a Fixed Linear Estimator

Before turning to the task of finding good algorithms, we first consider the more basic challenge of optimizing Equation 1: given a linear algorithm, how good is it?

As noted above, the matrix in the parentheses in the second expression of Equation 1 is positive semidefinite. In fact, for appropriate coefficients \(a_i\), we can make the matrix \(\frac{1}{m} \sum_{i=1}^{m} (a_i - b_i)^T (a_i - b_i)\) be an arbitrary positive semidefinite matrix (though possibly at the cost of an “unnatural” estimation algorithm). Thus the problem of computing or estimating the performance of an estimation algorithm is identical to what is known as the positive semidefinite Grothendieck problem.

**Definition 7.** The positive semidefinite Grothendieck problem, given an \(n \times n\) positive semidefinite matrix \(M\) is to evaluate:

\[
\max_{x_1, \ldots, x_n \in \{-1, 1\}} x^T M x \tag{2}
\]

(Note that this problem is sometimes phrased as the optimization over a pair of vectors \(x, y\), of the expression \(x^T M y\), though for positive semidefinite \(M\), an optimum will always be attained when \(x = y\).)

The positive semidefinite Grothendieck problem includes MAX-CUT as a special case, since, for an undirected graph \(G\), its Laplacian \(L\) is positive semidefinite, and for any vector \(x \in \{-1, 1\}^n\) that labels its vertices, the value of \(x^T L x\) will equal the total degree of the graph plus the size of the cut induced by the labels of \(x\). Thus, since MAX-CUT is NP-hard, evaluating the performance of a fixed estimator is also NP-hard. Further, Håstad showed that it is NP-hard to even approximate MAX-CUT to within a multiplicative factor of \(\frac{17}{16}\) [10]. For the more general case of the semidefinite Grothendieck problem considered here, Khot and Naor showed the unique-games hardness of approximating the optimum to within a factor of \(\frac{\pi}{\sqrt{2}}\). For the more general case of the semidefinite Grothendieck problem considered here, Khot and Naor showed the unique-games hardness of approximating the optimum to within a factor of \(\frac{\pi}{\sqrt{2}}\); this result was recently strengthened by Briët, Regev, and Saket to show it is in fact NP-hard to get an approximation ratio better than \(\frac{\pi}{\sqrt{2}}\) [13, 1]. Thus, even for a fixed linear estimation algorithm, we cannot hope to approximate its performance—given by Equation 1—to within a factor of \(\frac{\pi}{\sqrt{2}}\).

**Approximation algorithms:** However, analogously to the Goemans-Williamson semidefinite relaxation of MAX-CUT, we consider the semidefinite relaxation of the semidefinite Grothendieck problem, replacing each scalar variable \(x_j\) with a vector \(v_j\) in the \(n\)-dimensional unit ball.
Definition 8. Given an \( n \times n \) positive semidefinite matrix \( M \), the semidefinite relaxation of the positive semidefinite Grothendieck problem is to evaluate:

\[
\max_{v_j \in \mathbb{R}^n : \|v_j\| \leq 1} \sum_{j,k=1}^{n} M(j,k) (v_j^T v_k)
\]

or, equivalently, letting “psd” denote the property of a matrix being positive semidefinite,

\[
\max_{v \text{ psd}, V(j,i) \leq 1} \sum_{j,k=1}^{n} M(j,k) V(j,k)
\]

Crucially, the set of positive semidefinite matrices is convex, so thus the optimization problem of Definition 8 (in its second form) maximizes a linear function over a convex set, and thus can be computed in polynomial time.

Goemans and Williamson famously showed, via a randomized rounding scheme, that the gap between MAX-CUT and the result of the induced positive semidefinite relaxation is bounded by a factor of 1.14 \[8\]. For the more general setting here, of arbitrary positive semidefinite matrices instead of graph Laplacians, Nesterov showed a bound of \( \frac{\pi}{2} \) \[16\]. We include a self-contained derivation here, for the sake of completeness.

Since scaling a single vector \( v_j \) affects Equation 3 in a convex quadratic manner, there will always be an optimum of Equation 3 where \( \|v_j\| = 1 \) for all \( j \). We assume this, for simplicity, when describing the randomized rounding procedure below.

Definition 9. Given \( n \) unit vectors \( v_j \in \mathbb{R}^n \), for \( j \in \{1, \ldots, n\} \), the Goemans-Williamson randomized rounding procedure chooses a random direction \( r \), and for each vector \( v_j \) returns a scalar \( x_j = \text{sign}(r^Tv_j) \).

Proposition 1. Given an \( n \times n \) positive semidefinite matrix \( M \), and \( n \) unit vectors \( v_1, \ldots, v_n \in \mathbb{R}^n \), the value of the relaxed Grothendieck problem, \( \sum_{j,k=1}^{n} M(j,k) (v_j^T v_k) \) is at most \( \frac{\pi}{2} \) times the expected value of the original Grothendieck problem evaluated on scalars \( x_1, \ldots, x_n \in [-1, 1] \) obtained from \( v_1, \ldots, v_n \) by the Goemans-Williamson randomized rounding procedure, \( \mathbb{E}[\sum_{j,k=1}^{n} M(j,k) x_j x_k] \).

Thus for any objective value that can be achieved in the relaxed problem, with vectors \( v_1, \ldots, v_n \), the original problem can achieve an objective value at least a \( \frac{2}{\pi} \) fraction of it, since it does so in expectation over scalars \( x_1, \ldots, x_n \) obtained by the randomized rounding procedure.

Proof of Proposition \[7\]. As in the analysis of the Goemans-Williamson randomized rounding scheme for MAX-CUT, the expected value \( \mathbb{E}[x_j x_k] = \mathbb{E}_r[\text{sign}(r^T v_j) \text{sign}(r^T v_k)] \), where \( r \) is a randomly chosen direction. Because of the rotational symmetry of the distribution of \( r \), we may equivalently rotate \( v_j \) and \( v_k \) into the plane, from which we can see that, for \( r \) also projected into the plane, \( \text{sign}(r^T v_j) \text{sign}(r^T v_k) \) equals 1 when \( r \) is within \( \frac{\pi}{2} \) radians of both \( v_j, v_k \) or neither of them. For a randomly chosen \( r \) in the plane, this happens with probability \( 1 - \frac{2}{\pi} \theta_{j,k} \), where \( \theta_{j,k} \) is the angle between \( v_j, v_k \), yielding that \( \mathbb{E}[x_j x_k] = 1 - \frac{2}{\pi} \theta_{j,k} \).

As \( \theta_{j,k} \) may be computed as \( \text{arccos}(v_j^T v_k) \), we may express the expected objective value after randomized rounding as

\[
\mathbb{E}\left[\sum_{j,k=1}^{n} M(j,k) x_j x_k\right] = \sum_{j,k=1}^{n} M(j,k) \left(1 - \frac{2}{\pi} \text{arccos}(v_j^T v_k)\right)
\]
Recall our overall aim, to show that this value times $\frac{\pi}{2}$ is greater than or equal to $\sum_{j,k=1}^{n} M(j,k)(v_j^T v_k)$. Subtracting these two quantities means that we need to show that the following quantity is non-positive:

$$\sum_{j,k=1}^{n} M(j,k)(v_j^T j_k - \frac{\pi}{2} + \arccos(v_j^T v_k))$$

(4)

The power series expansion of $\arccos(y)$ starts $\arccos(y) = \frac{\pi}{2} - y + \sum_{\ell \geq 3} c_{\ell} y^\ell$ where all the remaining coefficients $c_{\ell}$ are nonpositive, and converges on the entire interval $y \in [-1, 1]$. Thus Equation (4) equals

$$\sum_{j,k=1}^{n} \left( M(j,k) \sum_{\ell \geq 3} c_{\ell}(v_j^T j_k)^\ell \right)$$

(5)

Since the matrix with $(j, k)$ entry $v_j^T v_k$ is positive semidefinite for any vectors $v_1, \ldots, v_n$, and since elementwise raising a positive semidefinite matrix to a positive integer power yields another positive semidefinite matrix, Equation (5) can be reexpressed as $\sum_{\ell \geq 3} \sum_{j,k=1}^{n} M(j,k) N^{(\ell)}(j,k)$ for some negative semidefinite matrices $N^{(\ell)}$, which is thus clearly less than or equal to 0, as desired.

Combining the lower bounds and upper bounds of this section immediately yields a tight characterization of the complexity of our task:

**Proposition 2.** Given a training/test distribution $P = (A_1, B_1), \ldots, (A_m, B_m)$, the problem of evaluating the performance $p$ of a linear estimation algorithm specified by vectors $a_1, \ldots, a_m \in \mathbb{R}^n$ is NP-hard to estimate to within a multiplicative factor of $\frac{\pi}{2}$. However, letting $M = \frac{1}{m} \sum_{i=1}^{m} (a_i - b_i)^T (a_i - b_i)$, the optimum of the convex program

$$\max_{V_{psd}, V_{(i,j)} \leq 1} \sum_{j,k=1}^{n} M(j,k) V(j,k)$$

(6)

is in the interval $[p, \frac{\pi}{2} p]$, and can be found in polynomial time by standard convex programming algorithms.

### 3 Computing a Near-Optimal Linear Estimator

While in Section 2.2 we analyzed the problem of evaluating the performance of a fixed linear estimator, here by contrast we aim to find a near-optimal linear estimator. This is a challenging setting for optimization, as even evaluating the objective function, to within a factor of $\frac{\pi}{2}$, is NP-hard (as discussed in Section 2.2). However, as we will see, the convex (semidefinite) relaxation derived in Section 2.2 not only lets us approximate the performance of a fixed algorithm to a $\frac{\pi}{2}$ factor, but also provides the crucial structure enabling us to find a linear estimator whose performance is within a $\frac{\pi}{2}$ factor of the best possible linear estimator.
Algorithm 1 $\frac{\pi}{2}$-approximation to the best linear estimator

**Input:** a joint distribution of training and test sets, expressed as a list $(A_1, b_1), \ldots, (A_m, b_m)$, where each $A_i \subset \{1, \ldots, n\}$ is the indices of the training set in the $i^{th}$ case, and each $b_i$ is a vector with uniform values over the test set in the $i^{th}$ case, as in Definition 4.

For an $n \times n$ matrix $V$ and a set $A_i \in \{1, \ldots, n\}$, let $V_{A_i}$ denote $V$ restricted to the rows in $A_i$, and let $V_{A_i,A_i}$ denote $V$ restricted to both rows and columns in $A_i$.

1. Compute the concave maximization

   $$\hat{V} = \arg \max_{V \text{ psd}, V_{j,j} \leq 1} \sum_{i=1}^{m} b_i^T (V - V_{(A_i)} V_{(A_i)}^{-1} V_{(A_i)}) b_i$$

   (7)

2. For each $i \in \{1, \ldots, n\}$, let $a_i$ when restricted to the coordinates $A_i$ equal $\hat{V}_{(A_i)}^{-1} \hat{V}_{(A_i)} b_i$, and 0 on the remaining coordinates. **Output** $a_1, \ldots, a_m$.

The function inside the sum in Step 1 is concave as a function of the matrix $V$ (as we will see) after extending it via limits to cover the case when $V_{(A_i,A_i)}$ is singular, and thus can be optimized in polynomial time. Further, the inverse in Step 2 to compute the linear coefficients can be interpreted as a pseudoinverse $\hat{V}_{(A_i)}^{-1}$ in cases where it would otherwise be singular.

**Theorem 2.** Algorithm 1 given a description of the joint distribution of training and test sets $(A_1, b_1), \ldots, (A_m, b_m)$, will return coefficients for a linear estimator whose performance is within a $\frac{\pi}{2}$ factor of the best linear estimator, in polynomial time. The value of the objective function achieved by $\hat{V}$, divided by $m$, is the mean squared error of the estimator.

**Proof.** Proposition 2 describes a convex optimization problem to approximate to within a factor of $\frac{\pi}{2}$ the performance of an estimator specified by vectors $a_1, \ldots, a_m \in \mathbb{R}^n$. We thus consider optimizing Equation 6 over this choice (omitting the $\frac{1}{m}$ factor for convenience):

$$\min_{a_i : \{j : a_i(j) \neq 0\} \subseteq A_i} \max_{V \text{ psd}, V_{j,j} \leq 1} \sum_{i=1}^{m} \sum_{j,k=1}^{n} (a_i - b_i)_{(j)} (a_i - b_i)_{(k)} V_{(j,k)}$$

(8)

By Proposition 2 this minimum (if we can efficiently find it), will be within a factor of $\frac{\pi}{2}$ of the performance of the best linear estimator, and the vectors $a_1, \ldots, a_m$ that achieve this minimum will describe an estimator with this performance.

We proceed by invoking von Neumann’s minimax theorem.

**Fact 1.** Given a function $f(x,y)$ that is convex as a function of its first argument and concave as a function of its second argument, and given convex domains $X, Y$, at least one of which is bounded, then

$$\min_{x \in X} \max_{y \in Y} f(x,y) = \max_{y \in Y} \min_{x \in X} f(x,y)$$

The condition that “at least one of $X, Y$ is bounded” is a relaxation of the original minimax theorem, shown sufficient by Sion [13].
We observe now that all the conditions of the minimax theorem are satisfied by the expression in Equation 8. As a function of $a_i$, the expression being optimized is the quadratic form with coefficients specified by the positive semidefinite matrix $V$; thus the expression is a convex function of $a_i$, and since such functions are summed over all $i \in \{1, \ldots, m\}$, the expression is a convex function of all the vectors $a_1, \ldots, a_m$. Since the expression is linear in $V$, it is thus also concave as a function of $V$. Finally, the domains of the vectors $a_1, \ldots, a_m$, along with the matrix $V$ are both convex, and, since a positive semidefinite matrix must have each entry bounded by the size of the largest diagonal entry, the condition that $V$ has diagonal entries bounded by 1 induces the same bound on the size of all entries of $V$.

Thus we invoke the minimax theorem to conclude that the value of Equation 8 is unchanged if we reverse the order of the min and the max:

$$\max_{V \text{ psd}, V_{(j,j)} \leq 1} \min_{a_i: \{j: a_i(j) \neq 0\} \subseteq A_i} \sum_{i=1}^{m} \sum_{j,k=1}^{n} (a_i - b_i)(a_i - b_i)V_{(j,k)}$$

(9)

Crucially, now, the inner minimization is simply a sum of positive semidefinite quadratic forms in each of the vectors $a_1, \ldots, a_m$. Reexpressing the inner sum in vector notation as $(a_i - b_i)^T V (a_i - b_i)$, the gradient of this quadratic form with respect to $a_i$ equals $2V(a_i - b_i)$. Thus, subject to the constraint that $a_i$ can only be nonzero on coordinates in $A_i$, if there exists a vector $a_i$ such that $V(a_i - b_i) = 0$ on coordinates $A_i$, then this $a_i$ attains the minimum; and otherwise the minimum is $-\infty$. The solution for $a_i$, restricted to the coordinates $A_i$, is thus $V^{-1}_{(A_i, A_i)} V_{(A_i)} b_i$ (or, when $V_{(A_i, A_i)}$ is singular, $V^+_{(A_i, A_i)} V_{(A_i)} b_i$ is the least-squares solution). Plugging this $a_i$ into the quadratic form yields $b_i^T (V - V^T_{(A_i)} V^{-1}_{(A_i, A_i)} V_{(A_i)}) b_i$ for the inner minimization of the $i^{\text{th}}$ term of the objective function. Finally, because of the setup of the minimax theorem, this expression must be a concave function of $V$, letting us conclude that Algorithm 1 can in fact conduct the optimization in polynomial time, as desired.

(As a side note, directly proving the above objective function is concave is a bit strange; it is a consequence of the fact that for positive definite $V$, and vectors $x$, the expression $x^T M^{-1} x$ is convex as a function of both arguments, implying it is convex even when both arguments are affine functions of the optimization variables.)

4 A Sample-Efficient Algorithm for Near-Optimal Linear Estimators

While Algorithm 1 takes as input the entire description $(A_1, B_1), \ldots, (A_m, B_m)$ of the joint training/test distribution, such a description might be (1) unavailable in practice and/or (2) have support $m$ that is exponentially large. To address both cases, in this section we design an algorithm that achieves essentially the performance guarantees of Algorithm 1 (as given by Theorem 2), though relying only on sampling access to the training/test distribution. Algorithm 2 will run in time polynomial in $n$ and independent of the (possibly exponential) distribution description length $m$. 
Algorithm 2 Sampling algorithm to approximate the best linear estimator

**Input:** Accuracy parameter $\epsilon > 0$; $t$ random samples from the joint distribution of training and test sets, $(A_{s_1}, b_{s_1}), \ldots, (A_{s_t}, b_{s_t})$, where each $A_i \subset \{1, \ldots, n\}$ is the set of training set indices in the $i^{th}$ case and each $b_i$ is a vector with uniform values over the test set in the $i^{th}$ case as in Definition 4; and the actual instance to predict, specified by $(A, b, x_A)$.

For an $n \times n$ matrix $V$ and a set $A_i \in \{1, \ldots, n\}$, let $V_{A_i}$ denote $V$ restricted to the rows in $A_i$, and let $V_{A_i, A_i}$ denote $V$ restricted to both rows and columns in $A_i$.

1. Compute the concave maximization

   $$\hat{V} = \arg\max_{V \succeq \epsilon, V_{j,j} \leq 1} \sum_{i=1}^{t} b_i^T (V - V_{(A_{s_i})} V_{(A_{s_i})}^{-1} V_{(A_{s_i})}) b_i$$

   (10)

2. Output the estimate $x_A \hat{V}_{(A)}^{-1} \hat{V}_{(A)} b$.

As compared with Algorithm 1, Algorithm 2 restricts the domain of optimization to matrices $V$ that have eigenvalues at least $\epsilon$, instead of at least 0 (which is a convex restriction). Crucially, instead of summing over all $m$ possible training/test set possibilities, the optimization is over a small subset of size $t$, obtained by sampling. Finally, the output of this algorithm is phrased as a single estimate for the data in question (described to the algorithm via the triple $A, b, x_A$, as opposed to Algorithm 1 which returned the entire list of $m$ linear estimator coefficients). The following theorem, characterizing the performance of the above algorithm, immediately implies Theorem 1.

**Theorem 3.** The mean squared error of the estimate output by Algorithm 2 over the randomness of the queried training and test sets $(A, b)$, is within a multiplicative $\frac{\pi}{2}$ factor and an additive $6\epsilon$ factor of the performance of the optimum linear estimator, with probability $1 - e^{-t \cdot \epsilon^5 / \text{poly}(n)}$ over the sampled inputs $(A_{s_1}, b_{s_1}), \ldots, (A_{s_t}, b_{s_t})$. The probability of failure can thus be made exponentially small in $n$ by using $t = \text{poly}(n) / \epsilon^5$ samples, for a sufficiently large polynomial in $n$.

We first prove three structural lemmas that characterize the optimization objective, and then put the pieces together making use of concentration bounds, applied over an $\epsilon$-net of matrices in the domain of the optimization.

**Lemma 1.** For any valid $V$, the $i^{th}$ term in the sum of Equation 7—or equivalently Equation 9 or Equation 10—is between 0 and 1.

**Proof.** From the derivation of Equation 7 in the proof of Theorem 2, the inner summation is equal to the inner minimization in Equation 9 which we analyze instead. Since the quadratic form specified by $V$ in Equation 9 is positive semidefinite, it thus always evaluates to a nonnegative number proving the first part of the claim.

Consider the inner minimum when all coefficients $a_i$ are identically 0. Since each $b_i$ is a non-negative vector of sum 1, and thus since all entries of $V$ have magnitude at most 1 (because of the diagonal constraint, and the positive semidefinite constraint), we have $\sum_{j,k=1}^{n} b_i(j) b_i(k) V_{j,k} \leq 1$, as desired. \qed
Lemma 2. The optimum objective value of the max in Equation 7 decreases by at most \( \epsilon \)m if the domain of the maximization is further restricted so that \( V \), instead of being positive semidefinite, must now have all eigenvalues at least \( \epsilon \).

Proof. From the derivation of Equation 7 in the proof of Theorem 2, the inner summation is equal to the inner minimization in Equation 9 which we analyze instead.

Letting \( V \) be the optimal matrix in Equation 9 we instead consider the matrix \( V_\epsilon = \epsilon I_n + (1 - \epsilon)V \) where \( I_n \) is the \( n \times n \) identity matrix. Since the objective is linear in \( V \), when evaluated at \( V_\epsilon \) it will have value \( \epsilon \) times the objective value for \( I_n \)—which is nonnegative by Lemma 1—plus \((1 - \epsilon)\) times its optimal objective value at \( V \)—which is at most 1 by Lemma 1. Thus \( V_\epsilon \) has objective value within \( \epsilon \) of the optimum, as desired.

Lemma 3. For a fixed symmetric matrix \( V \) whose eigenvalues are all at least \( \epsilon \), the expression inside the sum of Equation 7, for any \( i \), varies with respect to changing a coordinate of \( V \) by at most \( \frac{d}{dV_{j,k}} b_i^T (V - V_{(A_i,A_i)}^{-1}) V_{(A_i,A_i)} b_i \leq \frac{1}{\epsilon^2} \text{poly}(n) \).

Proof. Since \( V \) has eigenvalues at least \( \epsilon \), so does any (principal) submatrix \( V_{(A_i,A_i)}^{-1} \). Thus the inverse \( V_{(A_i,A_i)}^{-1} \) has eigenvalues at most \( \frac{1}{\epsilon^2} \), and thus the \( L_2 \) norm of any column of \( V_{(A_i,A_i)}^{-1} \) is at most \( \frac{1}{\epsilon^2} \). Since \( \frac{d}{dV_{j,k}} V_{(A_i,A_i)}^{-1} \) equals negative the inner product of the columns (or rows) \( j \) and \( k \) of \( V_{(A_i,A_i)}^{-1} \), this derivative is thus at most \( \frac{1}{\epsilon^2} \). Applying the product rule can increase this by only a \( \text{poly}(n) \) factor.

We assemble these pieces to prove the performance of Algorithm 2.

Proof of Theorem 3. For any fixed \( V \) in Equation 7 the average of the \( m \) terms in the sum may be estimated as the empirical average of the \( t \) terms we can compute from our randomly sampled inputs \((A_s, b_s), \ldots, (A_s, b_s)\). Since, by Lemma 2 each term is between 0 and 1, the standard Chernoff/Hoeffding bounds imply that the empirical mean of \( t \) random terms will be within \( \epsilon \) of the true mean except with probability \( e^{-2\epsilon^2t} \).

Let \( \epsilon' = \epsilon^3 / \text{poly}(n) \) be a radius such that, by Lemma 2, any two matrices satisfying the constraints of the arg max of Equation 10 that are within distance \( \epsilon' \) of each other must yield values for each term in the sum, that are within \( \epsilon \) of each other. Consider applying the concentration bounds of the previous paragraph to each \( V \) in an \( \epsilon' \)-net of matrices satisfying the conditions of Equation 10—namely, positive definite with eigenvalues at least \( \epsilon \), and all diagonal entries at most 1. Recall that an \( \epsilon' \)-net will have each matrix within distance \( \epsilon' \) of one of the matrices in the net, and that the net will consist of \( e^{\text{poly}(n)/\epsilon'} \) matrices. As we consider bounds up to \( \text{poly}(n) \) factors, the choice of norm for the matrices does not matter, but for concreteness, consider the \( \epsilon' \)-net to be defined in the Frobenius norm. By the union bound, the Chernoff/Hoeffding bound of the previous paragraph applies for every \( V \) in the \( \epsilon' \)-net except with probability \( e^{-2\epsilon^2t + \text{poly}(n)/\epsilon'} \), which is thus negligible when the number of samples is \( t = \text{poly}(n)/\epsilon' \) factors.

We thus show that the performance of the estimator described by the sampled \( \hat{V} \) is close to the performance of the optimal linear estimator \( \hat{V} \) with eigenvalues at least \( \epsilon \). Let \( \hat{V}', \hat{V}' \) respectively represent the nearest elements of the \( \epsilon' \)-net to \( \hat{V}, \hat{V} \) respectively. For ease of notation, we let \( \hat{f}(\hat{V}) \) and \( \hat{f}(\hat{V}) \) respectively describe the functions of \( V \) described by the average term in the sums of Equations 7 and 10 respectively. Thus we have

\[
\hat{f}(\hat{V}) \geq \hat{f}(\hat{V}') - \epsilon \geq \hat{f}(\hat{V}') - 2\epsilon \geq \hat{f}(\hat{V}) - 3\epsilon \geq \hat{f}(\hat{V}') - 3\epsilon \geq \hat{f}(\hat{V}') - 4\epsilon \geq \hat{f}(\hat{V}) - 5\epsilon,
\]
where the inequalities hold respectively because of (1) the $\epsilon'$-nearness of $\tilde{V}, \tilde{V}'$ combined with the derivative guarantee of Lemma 3 as applied to $\tilde{f}$; (2) the Chernoff/Hoeffding bound at the point $\tilde{V}'$ of the $\epsilon'$-net; (3) the $\epsilon'$-nearness of $\tilde{V}, \tilde{V}'$ combined with the derivative guarantee of Lemma 3 as applied to $\tilde{f}$; (4) the fact that $\tilde{V}$ attains the maximum of $\tilde{f}$; (5) the Chernoff/Hoeffding bound at the point $V'$ of the $\epsilon'$-net; and (6) the $\epsilon'$-nearness of $\tilde{V}, V'$ combined with the derivative guarantee of Lemma 3 as applied to $\tilde{f}$.

Thus, the algorithm described by $\tilde{V}$ has true performance within $5\epsilon$ of the optimal under the eigenvalue constraint, achieved by $\hat{V}$. By Lemma 2, $\hat{V}$ itself is within $\epsilon$ of the true optimal performance of Equation 7, which in turn is within a factor of $\frac{\pi}{2}$ of that of the best linear estimator, as desired.

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