

Learning Single Index Models in High Dimensions

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Abstract

Single Index Models (SIMs) are simple yet flexible semi-parametric models for classification and regression. Response variables are modeled as a nonlinear, monotonic function of a linear combination of features. Estimation in this context requires learning both the feature weights, and the nonlinear function. While methods have been described to learn SIMs in the low dimensional regime, a method that can efficiently learn SIMs in high dimensions has not been forthcoming. We propose three variants of a computationally and statistically efficient algorithm for SIM inference in high dimensions. We establish excess risk bounds for the proposed algorithms and experimentally validate the advantages that our SIM learning methods provide relative to Generalized Linear Model (GLM) and low dimensional SIM based learning methods.

1 Introduction

High-dimensional learning is often tackled using generalized linear models, where we assume that a response variable $Y \in \mathbb{R}$ is related to a feature vector $X \in \mathbb{R}^d$ via

$$\mathbb{E}[Y|X = \mathbf{x}] = g_*(\mathbf{w}_*^\top \mathbf{x}) \quad (1)$$

for some weight vector $\mathbf{w}_* \in \mathbb{R}^d$ and some monotonic and smooth function g_* called the transfer function. Typical examples of g_* are the logit function and the probit function for classification, and the linear function for regression. While classical work on generalized linear models (GLMs) assumes g_* is known, this potentially nonlinear function is often unknown and hence a major challenge in statical inference.

The model in (1) with g_* unknown is called a *Single Index Model (SIM)* and is a powerful semi-parametric generalization of a GLM. SIMs were first introduced in econometrics and statistics [3, 4, 2]. Recently, computationally and statistically efficient algorithms have been provided for learning SIMs [6, 5] in low-dimensional settings where the number of samples/observations n is larger than the ambient dimension d . However, modern data analysis problems in machine learning, signal processing, and computational biology involve high dimensional datasets, where the number of parameters far exceeds the number of samples ($n \ll d$).

In this paper we consider the problem of learning SIMs, given labeled data, in the *high-dimensional* regime. We provide algorithms that are both computationally and statistically efficient for learning SIMs in high-dimensions, and validate our methods on several high dimensional datasets. Our contributions in this paper can be summarized as follows:

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1. We propose a suite of algorithms to learn SIMs in high dimensions. Our simplest algorithm called SILO (Single Index Lasso Optimization) is a simple, non iterative method that estimates the vector \mathbf{w}_* and a monotonic, Lipschitz function g_* . iSILO and ciSILO are iterative variants of SILO that use different loss functions. While iSILO uses a squared loss function, ciSILO uses a calibrated loss function that adapts to the SIM from which our data is generated.
2. We provide excess risk bounds on the hypotheses returned by SILO, iSILO, ciSILO.
3. We experimentally compare our algorithms with other methods used both for SIM learning and high dimensional parameter estimation on various real world high dimensional datasets. Our experimental results show superior performance of iSILO and ciSILO when compared to commonly used methods for high dimensional estimation.

The rest of the paper is organized as follows: In Section (2), we formally set up the problem we wish to solve, and detail the proposed methods, SILO, iSILO, ciSILO. In Section (3), we perform a theoretical analysis of SILO, iSILO, and ciSILO. We perform a thorough empirical evaluation on several datasets in Section (4), and conclude our paper in Section (5). Full proofs of our theoretical analysis are available in the appendix.

1.1 Related work

High dimensional parameter estimation for GLMs has been widely studied, both from a theoretical and algorithmic point of view ([15, 7, 9] and references therein). Learning SIMs is a harder problem and was first introduced in econometrics [4] and statistics [3]. In [6] the authors proposed and analyzed the Isotron algorithm to learn SIMs in the low dimensional setting. Isotron uses perceptron type updates to learn \mathbf{w}_* , along with application of the Pool Adjacent Violator (PAV) algorithm to learn g_* . This was improved in [5] where the authors proposed the Slisotron algorithm that combined perceptron updates to learn \mathbf{w}_* along with a Lipschitz PAV (LPAV) procedure to learn g_* . Both the Isotron and the Slisotron algorithm rely on performing perceptron updates. While the perceptron algorithm works for low-dimensional classification problems, to the best of our knowledge the performance of the perceptron algorithm has not been studied in high-dimensions. Hence, it is not clear if the Isotron and the Slisotron algorithms designed for learning SIM in low-dimensions would work in the high dimensional setting.

Alquier and Biau [1] consider learning high dimensional single index models. The authors provide estimators of g_* , \mathbf{w}_* using PAC-Bayesian analysis. However, the estimator relies on reversible jump MCMC, and it is seemingly hard to implement. Also, the MCMC step is slow to converge even for moderately sized problems. To the best of our knowledge, simple, practical algorithms with theoretical guarantees and good empirical performance for learning single index models in high dimensions are not available. Restricted versions of the SIM estimation problem have been considered in [11, 12], where the authors are only interested in accurate parameter estimation and not prediction. Hence, in these works the proposed algorithms do not learn the transfer function.

The LPAV: Before we discuss algorithms for learning high dimensional SIMs, we discuss the LPAV algorithm proposed in [5], as an extension to the PAV method used in [6]. Given data $(p_1, y_1), \dots, (p_n, y_n)$, where $p_1, \dots, p_n \in \mathbb{R}$ the LPAV outputs the best univariate monotonic, 1-Lipschitz function \hat{g} , that minimizes squared error $\sum_{i=1}^n (g(p_i) - y_i)^2$. In order to do this, the LPAV first solves the following optimization problem:

$$\hat{\mathbf{z}} = \arg \min_{\mathbf{z} \in \mathbb{R}^n} \|\mathbf{z} - \mathbf{y}\|_2^2 \quad \text{s.t.} \quad 0 \leq z_j - z_i \leq p_j - p_i \text{ if } p_i \leq p_j \quad (2)$$

where $\hat{g}(p_i) = \hat{z}_i$. This gives us the value of \hat{g} on a discrete set of points p_1, \dots, p_n . To get \hat{g} everywhere else on the real line, we simply perform linear interpolation as follows: Sort p_i for all i and let $p_{\{i\}}$ be the i^{th} entry after sorting. Then, for any $\zeta \in \mathbb{R}$, we have

$$\hat{g}(\zeta) = \begin{cases} \hat{z}_{\{1\}}, & \text{if } \zeta \leq p_{\{1\}} \\ \hat{z}_{\{n\}}, & \text{if } \zeta \geq p_{\{n\}} \\ \mu \hat{z}_{\{i\}} + (1 - \mu) \hat{z}_{\{i+1\}} & \text{if } \zeta = \mu p_{\{i\}} + (1 - \mu) p_{\{i+1\}} \end{cases} \quad (3)$$

In the algorithms that we shall discuss in this paper we shall invoke the LPAV routine with p_i set to the projection of the data point \mathbf{x}_i on some algorithm-dependent weight vector \mathbf{w} .

2 Statistical model and proposed algorithms

Assume we are provided i.i.d. data $\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$, where the label Y is generated according to the model $\mathbb{E}[Y|X = \mathbf{x}] = g_*(\mathbf{w}_*^\top \mathbf{x})$ for an unknown parameter vector $\mathbf{w}_* \in \mathbb{R}^d$ $n \ll d$ and unknown 1-Lipschitz, monotonic function g_* . We additionally assume that $y \in [0, 1]$, $\|\mathbf{w}_*\|_2 \leq 1$ and $\|\mathbf{w}_*\|_0 \leq s$, where $\|\cdot\|_0$ is the ℓ_0 pseudo-norm. The sparsity assumption on \mathbf{w}_* is motivated by the fact that consistent estimation in high dimensions is an ill-posed problem without making further structural assumptions on the underlying parameters.

Our goal is to make predictions on unseen data. Specifically, we would like to provide estimators \hat{g} and $\hat{\mathbf{w}}$ of g_* and \mathbf{w}_* so that given a previously unseen sample \mathbf{x} , we predict $\hat{y} = \hat{g}(\hat{\mathbf{w}}^\top \mathbf{x})$. To this end, we propose three algorithms that we explain next

2.1 SILO: Single Index Lasso Optimization

We first propose SILO, a simple SIM learning algorithm that first learns $\hat{\mathbf{w}}$ and then fits a function \hat{g} using $\hat{\mathbf{w}}$. Specifically, SILO performs the following two steps in a single pass:

1. In order to learn $\hat{\mathbf{w}}$ we solve the problem that was first proposed in [10]. This optimization problem is independent of the transfer function g_* and minimizes a linear loss subject to model constraints:

$$\hat{\mathbf{w}} = \arg \min_{\substack{\mathbf{w}: \|\mathbf{w}\|_2 \leq 1, \\ \|\mathbf{w}\|_1 \leq \sqrt{s}}} -\frac{1}{n} \sum_{i=1}^n \mathbf{y}_i \mathbf{x}_i^\top \mathbf{w}. \quad (4)$$

where the constraint $\|\mathbf{w}\|_1 \leq \sqrt{s}$ arises from constraining an s -sparse vector to have unit Euclidean norm.

2. After learning $\hat{\mathbf{w}}$, SILO simply fits a 1-Lipschitz monotonic function by invoking the LPAV routine with the vector $\mathbf{p} = [p_1, \dots, p_n]$, where $p_i = \hat{\mathbf{w}}^\top \mathbf{x}_i$. LPAV outputs a function \hat{g} . Our final predictor has the form $\hat{y} = \hat{g}(\hat{\mathbf{w}}^\top \mathbf{x})$.

Note that there is no need to re-learn $\hat{\mathbf{w}}$ after learning \hat{g} , since the optimization problem to learn $\hat{\mathbf{w}}$ is independent of \hat{g} . This property makes SILO a very simple and a computationally attractive algorithm.

2.2 iSILO: Iterative SILO with squared loss

SILO is computationally very efficient, since it only involves learning $\hat{\mathbf{w}}, \hat{g}$ once. However, completely ignoring \hat{g} to learn $\hat{\mathbf{w}}$ could be suboptimal, and we propose two algorithms to overcome this drawback. We first propose iSILO, an iterative method detailed in Algorithm 1. Given the model in (1), iSILO minimizes the squared loss with a sparsity penalty to estimate $\hat{\mathbf{w}}, \hat{g}$:

$$\hat{\mathbf{w}}, \hat{g} = \arg \min_{\mathbf{w}, g} \frac{1}{n} \sum_{i=1}^n (y_i - g(\mathbf{w}^\top \mathbf{x}_i))^2 + \lambda \|\mathbf{w}\|_1. \quad (5)$$

We adopt an alternating minimization procedure. In iteration t , given g_{t-1} , we would ideally perform a proximal point update w.r.t. \mathbf{w} to obtain

$$\mathbf{w}_t = \text{Prox}_{\lambda\eta, \|\cdot\|_1} \left(\mathbf{w}_{t-1} - \frac{\eta}{n} \sum_{i=1}^n (g_{t-1}(\mathbf{w}_{t-1}^\top \mathbf{x}_i) - y_i) g'_{t-1}(\mathbf{w}_{t-1}^\top \mathbf{x}_i) \mathbf{x}_i \right)$$

where $\text{Prox}(\cdot)$ is the soft thresholding operator associated with the $\|\cdot\|_1$ norm, $\eta > 0$ is an appropriate step size, and g'_t is the derivative of g_t . Unfortunately, the above gradient step requires us to estimate the derivative of g_t , which can be difficult. So, instead of performing the above proximal gradient update, we instead perform a proximal perceptron type update similar in spirit to [6, 5], by replacing g'_{t-1} by the Lipschitz constant of g_{t-1} . Since g_{t-1} is obtained using

Algorithm 1: iSILO

Require: Data: $X = [\mathbf{x}_1, \dots, \mathbf{x}_n]$, Labels: $\mathbf{y} = [y_1, \dots, y_n]^\top$, Regularization: λ , Step size η , Initial parameters: g_0 is 1-Lipschitz, monotonic function, $\mathbf{w}_0 \in \mathbb{R}^d$, Iterations: $T > 0$.

- 1: Initialize $\hat{\mathbf{w}} = \mathbf{w}_0, \hat{g} = g_0$.
- 2: $\text{opterr} = \text{MSE}(\mathbf{w}_0, g_0)$
- 3: **for** $t=1, \dots, T$ **do**
- 4: Perform the update shown in Equation (6) to get \mathbf{w}_t .
- 5: Calculate $\text{err} = \text{MSE}(\mathbf{w}_t, g_{t-1})$.
- 6: **if** $\text{err} \leq \text{opterr}$ **then**
- 7: $\text{opterr} = \text{err}$.
- 8: $\hat{\mathbf{w}} = \mathbf{w}_t, \hat{g} = g_{t-1}$
- 9: **end if**
- 10: Obtain g_t by solving problem (2) with $p_i = \mathbf{w}_t^\top \mathbf{x}_i$ and linear interpolation (3)
- 11: Calculate $\text{err} = \text{MSE}(\mathbf{w}_t, g_t)$.
- 12: **if** $\text{err} \leq \text{opterr}$ **then**
- 13: $\text{opterr} = \text{err}$.
- 14: $\hat{\mathbf{w}} = \mathbf{w}_t, \hat{g} = g_t$
- 15: **end if**
- 16: **end for**
- 17: Output $\hat{\mathbf{w}}, \hat{g}$

the LPAV algorithm, g_{t-1} is 1-Lipschitz. Note that unlike the perceptron, we have a non unity step size. This leads to the following update equation

$$\mathbf{w}_t = \text{Prox}_{\lambda\eta, \|\cdot\|_1} \left(\mathbf{w}_{t-1} - \frac{\eta}{n} \sum_{i=1}^n (g_{t-1}(\mathbf{w}_{t-1}^\top \mathbf{x}_i) - y_i) \mathbf{x}_i \right) \quad (6)$$

Given \mathbf{w}_t in iteration t , iSILO updates g_t to be the solution to the LPAV problem with $p_i = \mathbf{w}_t^\top \mathbf{x}_i$.

The non-convexity of (5) requires us to perform a book-keeping procedure that keeps track of the best estimate of $\hat{g}, \hat{\mathbf{w}}$ by calculating the MSE of the current hypothesis on a held-out validation set. This is done in steps 5-9 and 12-16 of Algorithms 1. Similar book-keeping procedures have been used in the Isotron, and Slisotron algorithms of [6, 5].

2.3 ciSILO: Iterative SILO with calibrated loss

iSILO like the Slisotron algorithm [5] use a squared loss function and an approximate gradient descent method to estimate \mathbf{w}_* . These methods do not take into account the derivative of the estimate of the transfer function while taking gradient descent steps. We now propose ciSILO, a version of SILO that uses a *calibrated* loss function that adapts to the SIM that we are trying to learn.

Suppose g_* was known. Let $\Phi_* : \mathbb{R} \rightarrow \mathbb{R}$ be a function such that $\Phi_*' = g_*$. Since g_* is monotonically increasing, Φ_* is convex, and we can learn $\hat{\mathbf{w}}$ by solving the following convex program:

$$\hat{\mathbf{w}} := \frac{1}{n} \sum_{i=1}^n \Phi_*(\mathbf{w}^\top \mathbf{x}_i) - \mathbf{y}_i \mathbf{w}^\top \mathbf{x}_i + \lambda \|\mathbf{w}\|_1 \quad (7)$$

When the transfer function is linear, Φ_* is a quadratic function, and we obtain the standard Lasso problem that minimizes squared loss with ℓ_1 penalty. When the transfer function is the logit function, (7) reduces to sparse logistic regression. Modulo, the ℓ_1 penalty term the above objective is a sample version of the following stochastic optimization problem:

$$\min_{\mathbf{w}} \mathbb{E}[\Phi_*(\mathbf{w}^\top \mathbf{x}) - \mathbf{y} \mathbf{w}^\top \mathbf{x}]. \quad (8)$$

If $\Phi'_* = g_*$, then the optimal solution to the above problem corresponds to the single index model that satisfies $\mathbb{E}[Y|X = x] = g_*(\mathbf{w}_*^\top \mathbf{x})$. Hence the above *calibrated loss function* takes into account the transfer function g_* used in the SIM via Φ_* and automatically adapts to the SIM from which the data is generated. When g_* is unknown, we instead consider the following optimization problem:

$$\hat{\mathbf{w}}, \hat{g} = \arg \min_{\mathbf{w}, g} \frac{1}{n} \sum_{i=1}^n \Phi(\mathbf{w}^\top \mathbf{x}_i) - \mathbf{y}_i \mathbf{w}^\top \mathbf{x}_i + \lambda \|\mathbf{w}\|_1 \quad \text{s.t.} \quad g = \Phi' \in \mathcal{G} \quad (9)$$

where the set $\mathcal{G} = \{g : \mathbb{R} \rightarrow \mathbb{R} \text{ is a 1-Lipschitz, monotonic function}\}$. Note that the above optimization problem optimizes for g via its integral Φ . ciSILO solves the above optimization problem by iteratively minimizing for w, g . The pseudo-code for ciSILO is given in Algorithm 2. There are three key update procedures performed in each iteration of ciSILO, which we explain below:

In Step 4, ciSILO fixes g to g_{t-1} and performs one step of a proximal point update on the objective in problem (9) w.r.t. \mathbf{w} to get:

$$\mathbf{w}_t = \text{Prox}_{\lambda\eta, \|\cdot\|_1} \left(\mathbf{w}_{t-1} - \frac{\eta}{n} \sum_{i=1}^n (g_{t-1}(\mathbf{w}_{t-1}^\top \mathbf{x}_i) - y_i) \mathbf{x}_i \right). \quad (10)$$

This step is identical to the update step in iSILO except that the g'_{t-1} does not feature in this update. Thus, the proximal point steps using a calibrated loss function can be performed *exactly* unlike the proximal point steps in iSILO.

The use of a calibrated loss function brings with it another challenge: The LPAV procedure, which was designed to minimize the squared loss, can no longer be used in ciSILO to estimate g_* . ciSILO instead uses a novel quadratic program to efficiently estimate g_* . From the first order optimality conditions of the optimization problem (9) for \mathbf{w} at \mathbf{w}_t we get that the optimal function g_t should satisfy

$$\frac{1}{n} \sum_{i=1}^n (g_t(\mathbf{w}_t^\top \mathbf{x}_i) - y_i) \mathbf{x}_i + \lambda \boldsymbol{\beta}_t = 0, \quad \boldsymbol{\beta}_t \in \partial \|\mathbf{w}_t\|_1. \quad (11)$$

g_t is updated such that L.H.S. of (11) has the smallest possible norm. This can be cast as a quadratic program (QP) as follows: Define, $\mathbf{p} = [p_1, \dots, p_n]^\top$, where $p_i = \mathbf{w}_t^\top \mathbf{x}_i$ and $\mathbf{z} = [z_1, \dots, z_n]^\top$, where $z_i = g_t(p_i)$. Let $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_n]$ be a $d \times n$ data matrix. Let $\mathbf{q} = n\lambda\boldsymbol{\beta} - \mathbf{X}^\top \mathbf{y}$. Now, solve the problem

$$\begin{aligned} \min_{\mathbf{z}} \quad & \|\mathbf{X}^\top \mathbf{z} + \mathbf{q}\|_2^2 \\ \text{s.t.} \quad & 0 \leq z_i \leq 1 \quad \forall i \quad \text{and} \quad 0 \leq z_j - z_i \leq p_j - p_i \quad \text{if } p_i \leq p_j \end{aligned} \quad (12)$$

We call optimization problem (12) **QPFit**, which is different from the LPAV given that it is derived from optimizing a calibrated loss function, which could be very different from the squared loss.

2.4 Initializing iSILO and ciSILO

Since both iSILO and ciSILO are non-convex, alternating minimization procedures, a good initialization is key to achieving good performance. A simple initialization would be to choose \mathbf{w}^0 randomly and g^0 to be the identity function. However, we initialize both methods with $\hat{\mathbf{w}}, \hat{g}$ obtained by running the (efficient) SILO algorithm from Section 2.1. We demonstrate in the next section that this yields very good theoretical guarantees, as well as good empirical performance in Section 4.

Remarks : Like in iSILO we perform book-keeping steps in ciSILO too. Since obtaining exact or approximate gradients in iSILO and ciSILO are easy we use first order methods to solve for $\hat{\mathbf{w}}$. Using line search methods in ciSILO, to compute step sizes, would require evaluating the calibrated loss function. This can be computationally intensive, since we have access to the calibrated loss function only via its gradient. Hence, in iSILO, and ciSILO we use a fixed step size to perform our updates. Despite the use of fixed step size, we show empirically that iSILO is often as competitive and sometimes better at making predictions than GLM based methods with optimal step sizes, and ciSILO is significantly superior.

Algorithm 2: ciSILO

Require: Data: $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_n]$, Labels $\mathbf{y} = [y_1, \dots, y_n]^\top$, Regularization parameter λ , step size η , Initial parameters: $\mathbf{w}_0 \in \mathbb{R}^d, g_0 : \mathbb{R} \rightarrow \mathbb{R}$ is 1-Lipschitz, monotonic function.

- 1: Initialize $\hat{\mathbf{w}} = \mathbf{w}_0, \hat{g} = g_0$.
 - 2: $\text{opterr} = MSE(\mathbf{w}_0, g_0)$
 - 3: **for** $t=1, 2, \dots, T$ **do**
 - 4: Perform the update step shown in Equation (10) to obtain \mathbf{w}_t .
 - 5: Calculate $\text{err} = MSE(\mathbf{w}_t, g_{t-1})$.
 - 6: **if** $\text{err} \leq \text{opterr}$ **then**
 - 7: $\text{opterr} = \text{err}$.
 - 8: $\hat{\mathbf{w}} = \mathbf{w}_t, \hat{g} = g_{t-1}$
 - 9: **end if**
 - 10: Calculate: $\mathbf{p} \leftarrow \mathbf{X}\mathbf{w}_t, \beta \leftarrow \partial \|\mathbf{w}_t\|_1, \mathbf{q} \leftarrow n\lambda\beta - \mathbf{X}^\top \mathbf{y}$
 - 11: Obtain g_t by solving problem (12) and linear interpolation.
 - 12: Calculate $\text{err} = MSE(\mathbf{w}_t, g_t)$.
 - 13: **if** $\text{err} \leq \text{opterr}$ **then**
 - 14: $\text{opterr} = \text{err}$.
 - 15: $\hat{\mathbf{w}} = \mathbf{w}_t, \hat{g} = g_t$
 - 16: **end if**
 - 17: **end for**
 - 18: Output $\hat{\mathbf{w}}, \hat{g}$
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3 Theoretical analysis of SILO, iSILO and ciSILO

In this section, we analyze the excess risk of the predictors output by iSILO, and ciSILO. For a given hypothesis $\hat{h}(x) = \hat{g}(\hat{\mathbf{w}}^\top \mathbf{x})$, define $\text{err}(h) := \mathbb{E}(h(\mathbf{x}) - \mathbf{y})^2$. The excess risk is then defined as

$$\mathcal{E}(\hat{h}) := \text{err}(\hat{h}) - \text{err}(h_\star) = \mathbb{E}(\mathbf{y} - \hat{h}(\mathbf{x}))^2 - \mathbb{E}(\mathbf{y} - g_\star(\mathbf{w}_\star^\top \mathbf{x}))^2 \quad (13)$$

We first list the technical assumptions we make:

- A1. The data $\mathbf{x}_1, \dots, \mathbf{x}_n$ is sampled i.i.d. from the standard multivariate Gaussian distribution.
- A2. $\mathbb{E}[Y|X = x] = g_\star(\mathbf{w}_\star^\top \mathbf{x})$, and $0 \leq Y \leq 1$,
- A3. g_\star is monotonic and 1-Lipschitz,
- A4. $\|\mathbf{w}_\star\|_0 \leq s, \|\mathbf{w}_\star\|_2 \leq 1, \|\hat{\mathbf{w}}\|_0 \leq k$, and $k \ll d$.

We provide sketches of relevant results in this section, and refer the interested reader to the Appendix for detailed proofs. Our first main result is an excess risk bounds for SILO:

Theorem 1. *Let $\hat{h}(x) = \hat{g}(\hat{\mathbf{w}}^\top \mathbf{x})$ be the hypothesis output by SILO. Let $\theta = \mathbb{E}_{\mu \sim N(0,1)} g_\star(\mu) \mu > 0$. Then under assumptions A1-A4, the excess risk of the predictor \hat{h} is, with probability at least $1 - \delta$, bounded from above by*

$$\mathcal{E}(\hat{h}) = \tilde{O} \left(\frac{(s+k) \log(2d)}{\theta} \sqrt{\frac{s}{n}} + \frac{1}{\sqrt{\theta}} \left(\frac{s}{n} \right)^{\frac{1}{4}} \sqrt{(s+k) \log(2d)} \right) \quad (14)$$

where \tilde{O} hides factors that are poly-logarithmic in $n, d, \frac{1}{\delta}, s$ and k .

Proof Sketch: For notational convenience, denote by $\epsilon^2 = \frac{1}{\theta} \sqrt{\frac{Cs \log(2d/s)}{n}}$, where $C > 0$ is a universal constant. WLOG, we can assume that $\|\hat{\mathbf{w}}\|_0 \leq s$. Our assumption on the sparsity of $\hat{\mathbf{w}}$ is pretty lenient, and is most often satisfied in practice. Also, since $\hat{\mathbf{w}}$ is obtained from SILO, we have $\|\hat{\mathbf{w}}\|_2 \leq 1, \|\hat{\mathbf{w}}\|_1 \leq \sqrt{s}$. From a result of Plan and Vershynin [10, Corollary 3.1] (Lemma 4 in appendix), we know that $\|\mathbf{w}_* - \hat{\mathbf{w}}\|_2^2 \leq \epsilon^2$. The excess risk $\mathcal{E}(\hat{h})$ can be bounded as follows.

$$\begin{aligned} \mathcal{E}(\hat{h}) &= \mathbb{E}[(\hat{g}(\hat{\mathbf{w}}^\top \mathbf{x}) - y)^2 - (g_*(\mathbf{w}_*^\top \mathbf{x}) - y)^2] = \mathbb{E}(\hat{g}(\hat{\mathbf{w}}^\top \mathbf{x}) - g_*(\mathbf{w}_*^\top \mathbf{x}))^2 \\ &= \mathbb{E}(\hat{g}(\hat{\mathbf{w}}^\top \mathbf{x}) - \hat{g}(\mathbf{w}_*^\top \mathbf{x}) + \hat{g}(\mathbf{w}_*^\top \mathbf{x}) - g_*(\mathbf{w}_*^\top \mathbf{x}))^2 \\ &\leq 2(s+k)\epsilon^2 \log(2d) + 2 \mathbb{E}(\hat{g}(\mathbf{w}_*^\top \mathbf{x}) - g_*(\mathbf{w}_*^\top \mathbf{x}))^2 \text{ with probability at least } 1 - \delta \end{aligned}$$

where we used the fact that \hat{g} is 1-Lipschitz, and upper bounds on the expected suprema of a collection of Gaussian random variables. Next, we shall bound the R.H.S. of the above equation.

$$\begin{aligned} \mathbb{E}(\hat{g}(\mathbf{w}_*^\top \mathbf{x}) - g_*(\mathbf{w}_*^\top \mathbf{x}))^2 &\stackrel{(a)}{\leq} \mathbb{E}(\hat{g}(\mathbf{w}_*^\top \mathbf{x}) - y)^2 - \mathbb{E}(g_*(\mathbf{w}_*^\top \mathbf{x}) - y)^2 \\ &\stackrel{(b)}{\leq} \frac{1}{n} \sum_{i=1}^n (\hat{g}(\mathbf{w}_*^\top \mathbf{x}_i) - y_i)^2 - (g_*(\mathbf{w}_*^\top \mathbf{x}_i) - y_i)^2 + \tilde{O}\left(\frac{(s \log(2d))^{1/4}}{\sqrt{n}}\right) \end{aligned}$$

In inequality (a) we used a certain projection inequality for convex sets (see Lemma 1 in appendix). To obtain inequality (b) we replace the expected value quantities with their empirical versions, plus deviation terms. Via standard application of large deviation inequalities, it is possible to establish that these deviations are $\tilde{O}\left(\frac{(s \log(2d))^{1/4}}{\sqrt{n}}\right)$ (see Lemma 5 in appendix). The proof concludes by upper bounding the empirical term in the above equation using optimality of \hat{g} and properties of maxima of a collection of Gaussian random variables.

Our next result is an upper bound on the excess risk bounds of iSILO and ciSILO:

Theorem 2. *Suppose $\hat{g}, \hat{\mathbf{w}}$ are the outputs of SILO on our data. Let $\hat{h}(\mathbf{x}) = \hat{g}(\hat{\mathbf{w}}^\top \mathbf{x})$ be the hypothesis corresponding to these outputs. Let $h_*(\mathbf{x}) \stackrel{\text{def}}{=} g_*(\mathbf{w}_*^\top \mathbf{x})$. Now, let \hat{h}_T be the output of ciSILO obtained by using $\hat{g}, \hat{\mathbf{w}}$ as initializers. Then under the assumptions A1-A4, with high probability we can bound the excess risk of \hat{h}_T by*

$$\mathcal{E}(\hat{h}_T) \leq \tilde{O}\left(\frac{(s+k) \log(2d)}{\theta} \sqrt{\frac{s}{n}} + \frac{1}{\sqrt{\theta}} \left(\frac{s}{n}\right)^{\frac{1}{4}} \sqrt{(s+k) \log(2d)}\right) + \sqrt{\frac{s \log^2(2d+1)}{n}} + \sqrt{\frac{1}{n}}$$

where \tilde{O} hides factors that are poly-logarithmic in $n, d, \frac{1}{\delta}, s, k$. Moreover, the same excess risk guarantees hold for \hat{h}_T obtained by running iSILO.

Proof Sketch : From Theorem 1 we know that

$$\mathcal{E}(\hat{h}) = \text{err}(\hat{h}) - \text{err}(h_*) \leq \tilde{O}\left(\frac{(s+k) \log(2d)}{\theta} \sqrt{\frac{s}{n}} + \frac{1}{\sqrt{\theta}} \left(\frac{s}{n}\right)^{\frac{1}{4}} \sqrt{(s+k) \log(2d)}\right)$$

Using standard large deviation arguments (see Lemma 6 in appendix) we can claim that $|\text{err}(\hat{h}) - \widehat{\text{err}}(\hat{h})| = \tilde{O}\left(\sqrt{\frac{s}{n}}\right)$ with probability at least $1 - \delta$. This gives us

$$\begin{aligned} \widehat{\text{err}}(\hat{h}) &= \text{err}(\hat{h}) + \tilde{O}\left(\sqrt{\frac{s}{n}}\right) = \text{err}(h_*) + \text{err}(\hat{h}) - \text{err}(h_*) + \tilde{O}\left(\sqrt{\frac{s}{n}}\right) \\ &= \text{err}(h_*) + \tilde{O}\left(\frac{(s+k) \log(2d)}{\theta} \sqrt{\frac{s}{n}} + \frac{1}{\sqrt{\theta}} \left(\frac{s}{n}\right)^{\frac{1}{4}} \sqrt{(s+k) \log(2d)}\right) + \sqrt{\frac{s \log^2(2d+1)}{n}}. \end{aligned}$$

Now consider \hat{h}_T obtained by running either ciSILO or iSILO for T iterations, when initialized with $\hat{\mathbf{w}}, \hat{g}$ obtained by running SILO first on the data. Since \hat{h}_T is chosen by using a held-out validation set as the iterate corresponding

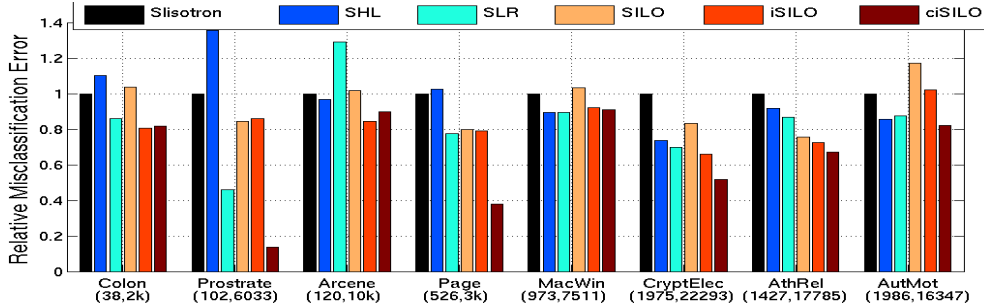


Figure 1: Errors rates are normalized so that the Slisotron has an error of 1. Note that ciSILO consistently outperforms all other methods, and iSILO is very competitive. The numbers below each dataset refer to (n, d)

to the smallest validation error, we can claim via Hoeffding inequality that the empirical error of \hat{h}_T cannot be too much larger than that of \hat{h} (for otherwise \hat{h}_T will not be the iterate with the smallest validation error). Precisely, if the validation set is of size n , then with high probability $\widehat{\text{err}}(\hat{h}_T) \leq \widehat{\text{err}}(\hat{h}) + \tilde{O}\left(\frac{1}{\sqrt{n}}\right)$. Using the above inequalities, and via standard large deviation arguments to bound $|\text{err}(\hat{h}_T) - \widehat{\text{err}}(\hat{h}_T)|$ we get the desired result.

Remarks : In the bound of Theorem 2, the first term in \tilde{O} dominates, and the excess risk bound is essentially $\tilde{O}\left(\frac{(s+k)\log(2d)}{\theta}\sqrt{\frac{s}{n}}\right)$. Also, using the output of SILO to initialize iSILO and ciSILO yields strong theoretical guarantees.

The constant θ in our results: θ acts like the signal to noise ratio in our results. The larger θ is, the better our bound gets. For example, for the logistic model, θ is approximately the norm of the data ($\sim \sqrt{\log(d)}$). For measurements of the form $\mathbf{y} = \text{sign}(\mathbf{x}^T \mathbf{w})$, θ is a constant. $\theta < 0$ can be easily tackled by reversing the signs of \mathbf{y} , and $\theta = 0$ implies that the data and observations are uncorrelated, and naturally any error bound will be meaningless.

Comparisons to existing results in low dimensions: In [5] the authors obtained dimension dependent as well as dimension independent bounds on the prediction error for the Slisotron algorithm for the SIM problem. However, these results were obtained under the restrictive assumption that $\|\mathbf{w}_*\|_2 \leq W$, $\|\mathbf{x}\|_2 \leq B$, and both W, B are fixed and independent of dimensions.¹ In order to carry through a correct high-dimensional analysis, one needs to let either W or B or both grow with d . In our analysis, we assume that the data is sampled from a standard multi-variate Gaussian, and hence $\|\mathbf{x}\|_2 \leq \sqrt{d}$ with high probability. If one were to replace B with \sqrt{d} in the results of [5], then the excess risk of their predictor would scale as $\min\left\{\frac{d}{n^{1/3}}, \frac{\sqrt{d}}{n^{1/4}}\right\}$, and since $d \gg n$, their bounds are meaningless in the high-dimensional setting. In contrast our results in Theorem 2 have a (poly)-logarithmic dependence on d , and hence are useful in the high dimensional setting studied in this paper. The same arguments apply to the results of [6], where in addition one needs a fresh batch of samples at each run.

4 Experimental results

We tested our algorithms SILO, iSILO, and ciSILO on many real world high dimensional datasets. For comparison with methods that assume g known, we used Sparse Logistic Regression (SLR), and Sparse Squared Hinge Loss minimization (SHL) [13]². We also tested the Slisotron [5] algorithm designed for low-dimensional SIM. For each dataset we randomly chose 60% of the data for training, and 20% each for validation and testing. The parameters λ, η are chosen via validation. Mac-Win, Crypt-Elec, Atheism-Religion and Auto-Motorcycle are from the 20 Newsgroups

¹In their analysis $B = 1$.

²code downloaded from <http://www.cs.ubc.ca/~schmidtm/Software/L1General.html>

dataset. Arcene is from the NIPS challenge ³, and the Page dataset is obtained from the WebKB dataset [8] ⁴. Prostrate and Colon cancer datasets are available online ⁵.

Figure 1 shows the misclassification error obtained on the test set. We show results for 8 datasets of varying size. Additional results are available in the supplementary material. Since the datasets (and errors) are varied, we normalize the error rates so that the Slisotron has unit error. As we can see from these results, using the calibrated loss in ciSILO yields the best performance in all the datasets considered, except MacWin. iSILO is as good as or better than SLR in 6/8 cases. It is encouraging to note that iSILO and ciSILO do well despite not having the luxury of choosing optimal step sizes at each iteration. Finally, the relatively poor performance of SILO underlines the importance of iterative methods in the SIM learning setting.

5 Conclusions

In this paper, we introduced a suite of algorithms based on sparse parameter estimation for learning single index models in the high dimensional setting. We derived excess risk guarantees for the proposed methods. Our algorithm employing a calibrated loss and a novel quadratic programming method to fit the transfer function achieves superior results compared to standard high dimensional classification methods based on minimizing the logistic or the hinge loss. In the future we plan to investigate learning single index models with structural constraints other than sparsity such as low rank, group sparsity, and indeed other very general constraints.

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³<http://www.nipsfsc.ecs.soton.ac.uk/datasets/>

⁴<http://vikas.sindhwani.org/manifoldregularization.html>

⁵<http://www.stat.cmu.edu/~jiashun/Research/software/HCClassification/Prostate/>

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A Preliminaries

We shall need a few definitions and a few important lemmas and propositions before we can state the proofs of our theorems. We shall consider the following function class.

$$\mathcal{G} = \{g : [-W, W] \rightarrow [0, 1], g \text{ is 1-Lipschitz and monotonic}\}. \quad (15)$$

Though the above definition of \mathcal{G} uses an unspecified parameter W , most often we shall use $W = \sqrt{s \log(2d)}$. The following result concerning suprema of a collection of i.i.d. Gaussian random variables is standard and we shall state it without proof.

Proposition 1. *Let $[g_i]_{i=1}^m$ be a collection of m i.i.d. Gaussian random variables with mean 0 and variance σ^2 . Then,*

$$\max_{i \in [m]} |g_i| \leq \sigma \left(\sqrt{\log(2m)} + \sqrt{2 \log(2/\delta)} \right) \quad \mathbf{w.p.} \geq 1 - \delta$$

The next lemma is standard and a proof can be found in Lemma 9 in [5].

Lemma 1. *Let \mathcal{F} be a convex class of functions, and let $f^* = \arg \min_{f \in \mathcal{F}} \mathbb{E}(f(x) - y)^2$. Suppose that $\mathbb{E}[Y|X = x] = g_*(\mathbf{w}_*^\top \mathbf{x})$ for some $g_* \in \mathcal{G}$. Then for any $f \in \mathcal{F}$, the following holds true*

$$\mathbb{E}[(f(x) - y)^2] - \mathbb{E}[(f(x) - y^*)^2] \geq \mathbb{E}[(f(x) - f^*(x))^2] \quad (16)$$

Lemma 2. *Let $\mathbf{x} \in \mathbb{R}^d$ be a standard normal random vector. Then with probability at least $1 - \delta$*

$$\mathbf{w}_*^\top \mathbf{x} \leq \tilde{O}(\sqrt{s \log(2d)})$$

Proof. The proof follows immediately from Proposition (1) and the fact that $\|\mathbf{w}_*\|_1 \leq \sqrt{s}$. \square

Lemma 3. *Let $\mathbf{e} \in \mathbb{R}^d$ be such that $\|\mathbf{e}\|_0 \leq s + k$ and $\|\mathbf{e}\|_2 \leq \epsilon$. Let \mathbf{x} be a standard normal random vector. Then with probability at least $1 - \delta$*

$$\mathbf{e}^\top \mathbf{x} \leq \tilde{O}(\epsilon \sqrt{(s + k) \log(2d)})$$

Proof. Let $\mathbf{e} = [e_1, \dots, e_d]$. Similarly, let $\mathbf{x} = [x_1, \dots, x_d]$. We then have

$$\mathbf{e}^\top \mathbf{x} = \sum_{i=1}^d e_i x_i \quad (17)$$

$$\leq \max |x_i| \sum_{i=1}^d |e_i| \quad (18)$$

$$\stackrel{(a)}{\leq} \sqrt{\log(2d)} \sum_{i=1}^{s+k} |e_i| \quad \mathbf{w.p.} \geq 1 - \delta \quad (19)$$

$$\stackrel{(b)}{\leq} \epsilon \sqrt{(s + k) \log(2d)}. \quad (20)$$

In obtaining inequality (a) we used the fact that the max of the absolute value of d Gaussian random variables is bounded by $\sqrt{\log(2d)}$. In equality (b) we used the fact that $\|\mathbf{e}\|_0 \leq s + k$, and hence only $s + k$ of the elements of \mathbf{e} are non-zero. \square

We next need the following important result (Corollary 3.1 in [10])

Lemma 4. *Let $\mathcal{W} = \{\mathbf{w} \in \mathbb{R}^d : \|\mathbf{w}\|_2 \leq 1, \|\mathbf{w}\|_1 \leq \sqrt{s}\}$. Let $\hat{\mathbf{w}}$ be obtained from SILO, shown in the main paper. Suppose, $\hat{\mathbf{w}} \in \mathcal{W}$. Let $\mathbf{x}_1, \dots, \mathbf{x}_n$ be n independent Gaussian random vectors. Assume that the measurements $\mathbb{E}[Y|X = x] = g_*(\mathbf{w}_*^\top \mathbf{x})$, where $\|\mathbf{w}_*\|_2 \leq 1, \|\mathbf{w}_*\|_0 \leq s$. Then with probability at least $1 - \delta$, the solution $\hat{\mathbf{w}}$ obtained from SILO satisfies the inequality*

$$\|\hat{\mathbf{w}} - \mathbf{w}_*\|_2^2 \leq \epsilon^2 \leq \frac{1}{\theta} \sqrt{\frac{Cs \log(2d/s)}{n}},$$

where $C > 0$ is a universal constant, and $\theta = \mathbb{E}_{\mu \sim N(0,1)} g_*(\mu) \mu$

Lemma 5. *With probability at least $1 - \delta$*

$$\mathbb{E}(\hat{g}(\mathbf{w}_*^\top \mathbf{x}) - y)^2 - \mathbb{E}(g_*(\mathbf{w}_*^\top \mathbf{x}) - y)^2 \leq \frac{1}{n} \sum_{i=1}^n (\hat{g}(\mathbf{w}_*^\top \mathbf{x}_i) - y_i)^2 - (g_*(\mathbf{w}_*^\top \mathbf{x}_i) - y_i)^2 + \tilde{O}\left(\sqrt{\frac{W}{n}}\right) \quad (21)$$

where \tilde{O} hides factors that are (poly)-logarithmic in $n, \frac{1}{\delta}$

Proof. From Lemma 6 (i) in [5] we know that

$$\mathcal{N}_2(r, \mathcal{G}, \mathbf{z}_1, \dots, \mathbf{z}_n) \leq \mathcal{N}_\infty(r, \mathcal{G}) \leq \frac{1}{r} 2^{\frac{2W}{r}}, \quad (22)$$

where $\mathcal{N}_2(r, \mathcal{G}, \mathbf{z}_1, \dots, \mathbf{z}_n)$ is the L_2 empirical covering number of function class \mathcal{G} at radius r , and $\mathcal{N}_\infty(r, \mathcal{G})$ is the L_∞ covering number. Using Dudley entropy integral, we can upper bound the empirical Rademacher complexity by

$$\hat{R}_n(\mathcal{G}) = \inf_{\alpha > 0} 4\alpha + 10 \int_\alpha^1 \sqrt{\frac{\log(1/r) + \frac{2W}{r}}{n}} dr \leq \frac{40\sqrt{W}}{\sqrt{n}}. \quad (23)$$

Hence, via standard large deviation inequalities we can claim that

$$\mathbb{E}[(\hat{g}(\mathbf{w}_*^\top \mathbf{x}) - y)^2] \leq \frac{1}{n} \sum (\hat{g}(\mathbf{w}_*^\top \mathbf{x}) - y)^2 + O\left(\sqrt{\frac{W}{n}}\right). \quad (24)$$

Similarly via standard concentration inequalities we can claim that with probability at least $1 - \delta$,

$$|\mathbb{E}[(g_*(\mathbf{w}_*^\top \mathbf{x}) - y)^2] - \frac{1}{n} \sum_i (g_*(\mathbf{w}_*^\top \mathbf{x}) - y)^2| \leq O\left(\sqrt{\frac{\log(2/\delta)}{n}}\right) \quad (25)$$

and hence putting together the above two inequalities the desired result follows. \square

B Proof of Theorem 1

For notational convenience, denote by $\epsilon^2 = \frac{1}{\theta} \sqrt{\frac{Cs \log(2d/s)}{n}}$, where $C > 0$ is a universal constant. Since, $\hat{\mathbf{w}}$ is obtained from SILO, we have $\|\hat{\mathbf{w}}\|_2 \leq 1, \|\hat{\mathbf{w}}\|_1 \leq \sqrt{s}$. The excess risk $\mathcal{E}(\hat{h})$ can be bounded as follows.

$$\begin{aligned} \mathcal{E}(\hat{h}) &= \mathbb{E}[(\hat{g}(\hat{\mathbf{w}}^\top \mathbf{x}) - y)^2 - (g_*(\mathbf{w}_*^\top \mathbf{x}) - y)^2] \\ &= \mathbb{E}(\hat{g}(\hat{\mathbf{w}}^\top \mathbf{x}) - g_*(\mathbf{w}_*^\top \mathbf{x}))^2 \\ &= \mathbb{E}(\hat{g}(\hat{\mathbf{w}}^\top \mathbf{x}) - \hat{g}(\mathbf{w}_*^\top \mathbf{x}) + \hat{g}(\mathbf{w}_*^\top \mathbf{x}) - g_*(\mathbf{w}_*^\top \mathbf{x}))^2 \\ &\leq 2 \mathbb{E}(\hat{g}(\hat{\mathbf{w}}^\top \mathbf{x}) - \hat{g}(\mathbf{w}_*^\top \mathbf{x}))^2 + 2 \mathbb{E}(\hat{g}(\mathbf{w}_*^\top \mathbf{x}) - g_*(\mathbf{w}_*^\top \mathbf{x}))^2 \\ &\stackrel{(a)}{\leq} 2 \mathbb{E}((\hat{\mathbf{w}} - \mathbf{w}_*)^\top \mathbf{x})^2 + 2 \mathbb{E}(\hat{g}(\mathbf{w}_*^\top \mathbf{x}) - g_*(\mathbf{w}_*^\top \mathbf{x}))^2 \\ &\stackrel{(b)}{\leq} 4s\epsilon^2 \log(2d) + 2 \mathbb{E}(\hat{g}(\mathbf{w}_*^\top \mathbf{x}) - g_*(\mathbf{w}_*^\top \mathbf{x}))^2 \text{ with probability at least } 1 - \delta \end{aligned} \quad (26)$$

Where in order to obtain inequality (a) we used the fact that \hat{g} is 1-Lipschitz, and in order to obtain inequality (b) we used Lemma (3). We shall now bound the R.H.S. of inequality 26. We do this as follows

$$\mathbb{E}(\hat{g}(\mathbf{w}_*^\top \mathbf{x}) - g_*(\mathbf{w}_*^\top \mathbf{x}))^2 \stackrel{(a)}{\leq} \mathbb{E}(\hat{g}(\mathbf{w}_*^\top \mathbf{x}) - y)^2 - \mathbb{E}(g_*(\mathbf{w}_*^\top \mathbf{x}) - y)^2 \quad (27)$$

$$\stackrel{(b)}{\leq} \frac{1}{n} \sum_{i=1}^n (\hat{g}(\mathbf{w}_*^\top \mathbf{x}_i) - y_i)^2 - (g_*(\mathbf{w}_*^\top \mathbf{x}_i) - y_i)^2 + \Delta_1 \quad (28)$$

In inequality (a) we used Lemma 1 with the function class $\mathcal{F} = \mathcal{G} \circ \mathbf{w}_*$. In inequality (b) we used Lemma (5) the expectation quantity in terms of its empirical quantity, with Δ_1 set to the maximum value of $\mathbf{w}_*^\top \mathbf{x}_i$. We know, from Lemma 2 that this max value is $\sqrt{s \log(2d)}$ with probability at least $1 - \delta$. Hence by substituting $W = \sqrt{s \log(2d)}$ for W , we get $\Delta_1 = O\left(\sqrt{\frac{\sqrt{s \log(2d)}}{n}}\right)$. Next we shall try to upper bound the empirical term in the above equation.

We have

$$\begin{aligned}
\frac{1}{n} \sum_{i=1}^n (\hat{g}(\mathbf{w}_*^\top \mathbf{x}_i) - y_i)^2 - (g_*(\mathbf{w}_*^\top \mathbf{x}_i) - y_i)^2 &= \frac{1}{n} \sum_{i=1}^n (\hat{g}(\hat{\mathbf{w}}^\top \mathbf{x}_i) - y_i - \hat{g}(\hat{\mathbf{w}}^\top \mathbf{x}_i) + \hat{g}(\mathbf{w}_*^\top \mathbf{x}_i))^2 - \\
&\frac{1}{n} \sum_{i=1}^n (g_*(\hat{\mathbf{w}}^\top \mathbf{x}_i) - y_i - g_*(\hat{\mathbf{w}}^\top \mathbf{x}_i) + g_*(\mathbf{w}_*^\top \mathbf{x}_i))^2 \\
&= \underbrace{\frac{1}{n} \sum_{i=1}^n (\hat{g}(\hat{\mathbf{w}}^\top \mathbf{x}_i) - y_i)^2 - \frac{1}{n} \sum_{i=1}^n (g_*(\hat{\mathbf{w}}^\top \mathbf{x}_i) - y_i)^2}_{\leq 0} \\
&\quad + \underbrace{\frac{1}{n} \sum_{i=1}^n (\hat{g}(\hat{\mathbf{w}}^\top \mathbf{x}_i) - \hat{g}(\mathbf{w}_*^\top \mathbf{x}_i))^2}_{T_1} - \underbrace{\frac{1}{n} \sum_{i=1}^n (g_*(\mathbf{w}_*^\top \mathbf{x}_i) - \hat{g}(\hat{\mathbf{w}}^\top \mathbf{x}_i))^2}_{\geq 0} \\
&\quad + \underbrace{\frac{2}{n} \sum_{i=1}^n (\hat{g}(\hat{\mathbf{w}}^\top \mathbf{x}_i) - y_i)(\hat{g}(\hat{\mathbf{w}}^\top \mathbf{x}_i) - \hat{g}(\mathbf{w}_*^\top \mathbf{x}_i))}_{T_2} \\
&\quad - \underbrace{\frac{2}{n} \sum_{i=1}^n (g_*(\hat{\mathbf{w}}^\top \mathbf{x}_i) - y_i)(g_*(\hat{\mathbf{w}}^\top \mathbf{x}_i) - g_*(\mathbf{w}_*^\top \mathbf{x}_i))}_{T_3} \tag{29}
\end{aligned}$$

where the term marked as ≤ 0 is negative because \hat{g} is the solution to a minimization problem that minimizes the empirical squared error under monotonicity and 1-Lipschitz constraints. Since g_* is also monotonic and 1-Lipschitz the squared error corresponding to the predictor $\hat{g}(\hat{\mathbf{w}}^\top \mathbf{x})$ should be smaller than the squared error corresponding to $g_*(\hat{\mathbf{w}}^\top \mathbf{x})$. The term marked as ≥ 0 is positive because it is an average of squared quantities. We shall now bound T_1, T_2, T_3 as follows

$$T_1 = \frac{1}{n} \sum_{i=1}^n (\hat{g}(\hat{\mathbf{w}}^\top \mathbf{x}_i) - \hat{g}(\mathbf{w}_*^\top \mathbf{x}_i))^2 \tag{30}$$

$$\stackrel{(a)}{\leq} \frac{1}{n} \sum_{i=1}^n ((\hat{\mathbf{w}} - \mathbf{w}_*)^\top \mathbf{x}_i)^2 \tag{31}$$

$$\stackrel{(b)}{\leq} (s + k) \epsilon^2 \log(2d) \tag{32}$$

where, to obtain inequality (a) we used the fact that \hat{g} is 1-Lipschitz, and to obtain inequality (b) we used Lemma 2.

To upper bound T_2 we proceed as follows

$$T_2 = \frac{2}{n} \sum_{i=1}^n (\hat{g}(\hat{\mathbf{w}}^\top \mathbf{x}_i) - y_i)(\hat{g}(\hat{\mathbf{w}}^\top \mathbf{x}_i) - \hat{g}(\mathbf{w}_*^\top \mathbf{x}_i)) \tag{33}$$

$$\stackrel{(a)}{\leq} \frac{2}{n} \sum_{i=1}^n |\hat{g}(\hat{\mathbf{w}}^\top \mathbf{x}_i) - \hat{g}(\mathbf{w}_*^\top \mathbf{x}_i)| \tag{34}$$

$$\stackrel{(b)}{\leq} \epsilon \sqrt{(s + k) \log(2d)} \tag{35}$$

To obtain inequality (a) we used the fact that $|y_i - \hat{g}(\hat{\mathbf{w}}^\top \mathbf{x}_i)| \leq 1$, and to obtain inequality (b) we used the fact that \hat{g} is 1-Lipschitz and Lemma 3. The same reasoning can be applied to upper bound T_3 to get $T_3 \leq \epsilon \sqrt{k \log(2d)}$.

Finally using lemma (4), we know that $\|\mathbf{w}_* - \hat{\mathbf{w}}\|_2^2 = \epsilon^2 \leq \tilde{O}(\frac{1}{\theta} \sqrt{\frac{s}{n}})$. Gathering all the terms, we get with probability at least $1 - \delta$,

$$\mathcal{E}(\hat{h}) = \tilde{O} \left(\frac{(s+k) \log(2d)}{\theta} \sqrt{\frac{s}{n}} + \frac{1}{\sqrt{\theta}} \left(\frac{s}{n} \right)^{\frac{1}{4}} \sqrt{(s+k) \log(2d)} \right) \quad (36)$$

where, $\theta = \mathbb{E}_{\mu \sim N(0,1)} g(\mu) \mu$ is a constant that depends on g_* .

C Large Deviation Guarantees for iSILO , ciSILO

Lemma 6. For any hypothesis $h(\mathbf{x}) = g(\mathbf{w}^\top \mathbf{x})$, where $\mathcal{W} = \{\mathbf{w} \in \mathbb{R}^d : \|\mathbf{w}\|_1 \leq \sqrt{s}, \|\mathbf{w}\|_2 \leq 1\}$, $g \in \mathcal{G}$, $\mathbf{w} \in \mathcal{W}$, we have

$$\text{err}(h_T) \leq \widehat{\text{err}}(h_T) + \tilde{O} \left(\sqrt{\widehat{\text{err}}(h_T)} \sqrt{\frac{s}{n}} \right),$$

where the \tilde{O} hides factors (poly) logarithmic in $d, n, 1/\delta$. In particular the above result also applies to h_T which is the hypothesis obtained by running iSILO or ciSILO for T iterations, and to \hat{h} , the hypothesis obtained by running SILO.

Before we give the proof of this theorem, we would like to point out that our assumption that $\hat{\mathbf{w}} \in \mathcal{W}$ is not at all restrictive. In practice the result provided by the iterates of a proximal gradient method used in SILO -M for a sufficiently large λ are sparse.

Proof. Consider the function class $\mathcal{H} = \{h(\mathbf{x}) = g(\mathbf{w}^\top \mathbf{x}) : \mathbf{w} \in \mathcal{W}, g \in \mathcal{G}\}$. By construction, we are guaranteed that $h_T, \hat{h} \in \mathcal{H}$, w.h.p., with $W = \sqrt{s \log(2d)}$. In order to establish a large deviation bound on the risk of h_T we shall first calculate the worst case Rademacher complexity of \mathcal{H} . To do this, we establish L_2 covering number of the function class \mathcal{H} by establishing L_∞ covering number of \mathcal{U} , and L_2 covering number of \mathcal{W} . Both these results are standard. From Lemma 6 in [5] we have

$$\mathcal{N}_\infty(\epsilon, \mathcal{G}) \leq \log \left(\frac{1}{\epsilon} \right) + \frac{2s \sqrt{\log(2d)}}{\epsilon}. \quad (37)$$

Since, $\|\mathbf{w}\|_1 \leq \sqrt{s}, \|\mathbf{x}\|_\infty \leq \tilde{O}(\sqrt{\log(2d)})$, we can use Theorem 3 in [16], to conclude that w.h.p.

$$\log \mathcal{N}_2(\mathcal{W}, \epsilon, n) \leq \frac{s \log^2(2d+1)}{\epsilon^2}. \quad (38)$$

It is not hard to see that

$$\log \mathcal{N}_2(\mathcal{F}, \epsilon, n) \leq \log \mathcal{N}_2 \left(\mathcal{W}, \frac{\epsilon}{2\sqrt{2}}, n \right) + \log \mathcal{N}_\infty \left(\mathcal{G}, \frac{\epsilon}{2\sqrt{2}} \right) \quad (39)$$

$$= \tilde{O} \left(\frac{s \log^2(2d+1)}{\epsilon^2} \right) \quad (40)$$

Using Lemma A.1 in [14] we can bound the worst case Rademacher complexity of \mathcal{H} by

$$\hat{R}_n(\mathcal{H}) \leq \tilde{O} \left(\sqrt{\frac{s \log^2(2d+1)}{n}} \right)$$

Finally applying Theorem 1 in [14] we get with probability at least $1 - \delta$

$$\text{err}(h_T) \leq \widehat{\text{err}}(h_T) + \tilde{O} \left(\sqrt{\widehat{\text{err}}(h_T)} \sqrt{\frac{s \log^2(2d+1)}{n}} \right).$$

□

D Proof of Theorem (2)

Proof. From Theorem (1) we know that

$$\mathcal{E}(\hat{h}) = \text{err}(\hat{h}) - \text{err}(h_*) \leq \tilde{O} \left(\frac{(s+k) \log(2d)}{\theta} \sqrt{\frac{s}{n}} + \frac{1}{\sqrt{\theta}} \left(\frac{s}{n}\right)^{\frac{1}{4}} \sqrt{(s+k) \log(2d)} \right) \quad (41)$$

Using Lemma 6 we can say that with probability at least $1 - \delta$

$$\widehat{\text{err}}(\hat{h}) = \text{err}(\hat{h}) + \sqrt{\frac{s \log^2(2d+1)}{n}} = \text{err}(h_*) + \text{err}(\hat{h}) - \text{err}(h_*) + \sqrt{\frac{s \log^2(2d+1)}{n}} \quad (42)$$

$$= \text{err}(h_*) + \tilde{O} \left(\frac{(s+k) \log(2d)}{\theta} \sqrt{\frac{s}{n}} + \frac{1}{\sqrt{\theta}} \left(\frac{s}{n}\right)^{\frac{1}{4}} \sqrt{(s+k) \log(2d)} \right) + \sqrt{\frac{s \log^2(2d+1)}{n}}. \quad (43)$$

Now consider \hat{h}_T obtained by running iSILO for T iterations, when initialized with \hat{w}, \hat{g} obtained by running SILO first on the data. Since \hat{h}_T is chosen by using a held-out validation set as the iterate corresponding to the smallest validation error, we can claim via Hoeffding inequality that the empirical error of \hat{h}_T cannot be too much larger than that of \hat{h} (for otherwise \hat{h}_T will not be the iterate with the smallest validation error). Precisely, if the validation set is of size n , then with high probability

$$\widehat{\text{err}}(\hat{h}_T) \leq \widehat{\text{err}}(\hat{h}) + \tilde{O} \left(\frac{1}{\sqrt{n}} \right). \quad (44)$$

Summing up Equations (41) and (42) we get

$$\widehat{\text{err}}(\hat{h}_T) \leq \text{err}(h_*) + \tilde{O} \left(\frac{(s+k) \log(2d)}{\theta} \sqrt{\frac{s}{n}} + \frac{1}{\sqrt{\theta}} \left(\frac{s}{n}\right)^{\frac{1}{4}} \sqrt{(s+k) \log(2d)} + \sqrt{\frac{s \log^2(2d+1)}{n}} + \sqrt{\frac{1}{n}} \right) \quad (45)$$

Now using Theorem (6) to upper bound $\text{err}(\hat{h}_T)$ in terms of $\widehat{\text{err}}(\hat{h}_T)$, and combining it with the above bound we get the desired result. The same arguments apply even to the ciSILO algorithm. □

E Additional Experimental Results

Here we report results on other high dimensional datasets. Figure 2 again shows the advantage of the calibrated, and iterative method ciSILO. Table 1 has the details of the datasets in Figure 2

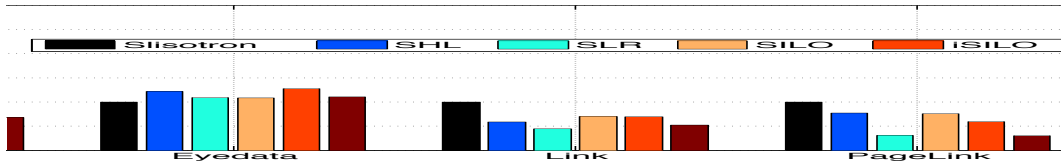


Figure 2: Comparison of different methods over different datasets. The results are normalized so that the Slisotron has error = 1

Dataset	n	d
Leukamia	44	7129
Eyedata	120	200
Link	526	1840
Page+Link	526	4840
Gisette	4200	5000

Table 1: Dataset details