Non-parametric Binary regression in metric spaces with KL loss

Ariel A vital, Klim Efremenko, Aryeh Kontorovich, David Toplin, Bo Waggoner
kish03@gmail.com, klim@bgu.ac.il, karyeh@cs.bgu.ac.il, david.tolpin@gmail.com, bwag@colorado.edu

October 21, 2020

Abstract

We propose a non-parametric variant of binary regression, where the hypothesis is regularized to be a Lipschitz function taking a metric space to [0, 1] and the loss is logarithmic. This setting presents novel computational and statistical challenges. On the computational front, we derive a novel efficient optimization algorithm based on interior point methods; an attractive feature is that it is parameter-free (i.e., does not require tuning an update step size). On the statistical front, the unbounded loss function presents a problem for classic generalization bounds, based on covering-number and Rademacher techniques. We get around this challenge via an adaptive truncation approach, and also present a lower bound indicating that the truncation is, in some sense, necessary.

1 Introduction

The algorithmic and statistical aspects of real-valued non-parametric regression are largely understood [Tsybakov, 2008, Györfi et al., 2002, Rasmussen and Williams, 2005]. At the opposite end of the spectrum is binary regression, where the dependent variable is \{0, 1\}-valued. Binary regression has numerous applications: consider, for example, predicting the number of defects in a production batch or a number of visitors of a web site in a time unit. A commonly used parametric latent variable model for binary regression is logistic regression. However, unlike Gaussian process regression, there is no known closed form efficient solution for logistic regression, even in the simplest linear setting. Non-parametric binary regression is a natural extension of linear logistic regression to cases where a non-linear dependency between predictors and the probability of outcome of 1 is desired. Non-parametric binary regression models have appeared in previous literature, [Hastie, 1983, Zhu and Hastie, 2002, Choudhuri et al., 2007], but, to our knowledge, rigorous statistical and computational aspects have not been thoroughly addressed.

In this work, we propose a variant of non-parametric binary regression which allows both an efficient approximation algorithm and a rigorous theoretical analysis. We consider the following problem setting:

Problem setting. Let \((X, \rho)\) be a metric space endowed with a distribution \(\mu\), and let \(h\) be a mapping \(h : X \to [0, 1]\). The learner observes \(n\) iid draws \((X_i, Y_i)\), where \((X_i, Y_i) \sim \mu\) Our goal is to estimate \(h\) point-wise using the sample, where the loss is defined in terms of Kullback-Liebler (KL) divergence:

\[
\ell(y, h(x)) = -y \ln(h(x)) - (1 - y) \ln(1 - h(x)).
\]

To make the problem well-posed (and to regularize against overfitting), we impose an \(L\)-Lipschitz condition on \(h\) with respect to the metric \(\rho\). This suggests a natural optimization problem: minimize the empirical risk under a smoothness constraint. Having chosen an optimal \(h\) on the labeled sample, we then Lipschitz-extend it to the whole space using standard techniques. As a technicality, we adaptively truncate \(h\) to keep it bounded away from 0 and 1; this enables fully empirical finite-sample guarantees, and also turns out to be, in some sense, necessary.
Our contributions. Aside from the conceptual problem setting, we provide several statistical and algorithmic results.

- an efficient algorithm (Algorithm 1) for solving the optimization problem implied by our learning setting: computing an \( L \)-Lipschitz \( h \) that minimizes the empirical risk with respect to the loss \( (1) \).
- a generalization bound (Theorem 6.1) based on covering numbers and an adaptive truncation
- a lower bound (Theorem 5.1, 5.2) indication that no non-trivial generalization bound is possible without some truncation.

2 Related Work

Non-parametric regression is well studied in a general setting [Simonoff, 1996, Györfi et al., 2002, Wasserman, 2006, Tsybakov, 2009]. Non-parametric binary regression has been employed in a number of works. [Hastie, 1983] gives a statistical recipe for binary regression using local logistic regression on spans over the predictor variable; references therein point to earlier works on non-linear and non-parametric binary regression.

A well-studied approach to non-parametric binary regression is Kernel logistic regression (KLR). [Zhu and Hastie, 2002] provides some results on KLR as well as literature overview. A different but related approach to non-parametric binary regression involves Gaussian process prior on the response probability function. [Choudhuri et al., 2007] gives a practical description of the method as long as overview of related prior research.

Interior point method (IPM) has vast literature. [Lesaja, 2009] gives a brief historical review of the development of IPM, wheres a short survey on the different variants can be found in [Glavic, 2004]. We’ve decided to stick to IPM as presented in [Nesterov, 2018], as it gives great detailed technical overview and complexity overview, while avoiding inner loops and line-searching. The first publication we’ve found to describe usage of IPM to solve Maximum-Likelihood appears in [Terlaky, 1995], discussing usage of both barrier method and primal-dual IPM. [Mizera, 2014] compares between EM and IPM schemes in the context of non-parametric maximum likelihood, where the latter performs better on the dual problem. [Kim et al., 2020] suggests a SQP approach for mixture proportions instead of IPM.

3 Technical Background

We write \( \ln \) for the natural logarithm and \( \log_b \) to specify a different base \( b \).

Metric spaces, Lipschitz constants. A metric \( \rho \) on a set \( \mathcal{X} \) is a symmetric function that is positive (except for \( \rho(x, x) = 0 \)) and satisfies the triangle inequality \( \rho(x, y) \leq \rho(x, z) + \rho(z, y) \); together the two comprise the metric space \( (\mathcal{X}, \rho) \). The diameter of a set \( A \subseteq \mathcal{X} \) is defined by \( \text{diam}(A) = \sup_{x, y \in A} \rho(x, y) \). There is no loss of generality in assuming \( \text{diam}(\mathcal{X}) = 1 \) since we can always scale the distances (when they are bounded). The Lipschitz constant of a function \( f : \mathcal{X} \to \mathbb{R} \), denoted \( \|f\|_{Lip} \) (or \( \|f\|_{Lip(\rho)} \) if we wish to make the metric explicit) is defined to be the smallest \( L \geq 0 \) such that \( |f(x) - f(y)| \leq L \rho(x, y) \) holds for all \( x, y \in \mathcal{X} \). In addition to the metric \( \rho \) on \( \mathcal{X} \), we will endow the space of all functions \( f : \mathcal{X} \to \mathbb{R} \) with the \( L_\infty \) metric:

\[
\|f - g\|_\infty = \sup_{x \in \mathcal{X}} |f(x) - g(x)|.
\]

A function is called \( L \)-Lipschitz if \( \|f\|_{Lip} \leq L \). We will denote by \( \mathcal{H}_L \) the collection of all \( L \)-Lipschitz functions \( \mathcal{X} \to [0,1] \). It will occasionally be convenient to restrict this class to
functions with \( \| f \|_{\text{Lip}} \geq 1 \); the latter collection will be denoted by \( H_{L \geq 1} \). This incurs no loss of generality in our results, as our Structural Risk Minimization procedure in general selects hypotheses whose Lipschitz constant grows with sample size. (See for example the risk bound presented at the beginning of Section 6.)

**Doubling dimension.** For a metric space \((X, \rho)\), let \( \lambda > 0 \) be the smallest value such that every ball in \( X \) can be covered by \( \lambda \) balls of half the radius. The **doubling dimension** of \( X \) is \( \text{ddim}(X) = \log_2 \lambda \). A metric space (or family of metrics) is called **doubling** if its doubling dimension is uniformly bounded.

Doubling metric spaces occur naturally in many data analysis applications, including for instance the geodesic distance of a low-dimensional manifold residing in a possibly high-dimensional space assuming mild conditions, e.g., on curvature. Some concrete examples for doubling metric spaces include: (i) \( \mathbb{R}^d \) for fixed \( d \) equipped with an arbitrary norm (ii) the planar earthmover metric between point sets of fixed size \( k \) [Gottlieb et al., 2014]; (iii) the \( n \)-cycle graph and its continuous version, the quotient \( \mathbb{R}/\mathbb{Z} \), and similarly bounded-dimensional tori.

**Self-concordance functions and barriers.** A function \( f \) is called self-concordant (s.c.) if there exists a constant \( M_f \geq 0 \) s.t. the following holds for all \( w \in \text{dom} f \) and \( u, v \in \mathbb{R}^n \):

\[
\langle f'''(w)[u]v, v \rangle \leq 2M_f \| u \|^3_w,
\]

where

\[
f'''(w) = \lim_{\alpha \to 0} \frac{1}{\alpha} \left[ \nabla^2 f(w + \alpha u) - \nabla^2 f(w) \right],
\]

and \( \| u \|_w \) is the primal local norm of \( f \), defined as

\[
\| u \|_w = \langle \nabla^2 f(w)u, u \rangle^{1/2}.
\]

In addition, we define the dual local norm as

\[
\| u \|_w^* = \langle (\nabla^2 f(w))^{-1}u, u \rangle^{1/2}.
\]

When the latter is applied to the gradient of \( f \), we have the so-called **local norm of the gradient**:

\[
\lambda_f(w) = \| \nabla f(w) \|_w^* = \langle (\nabla^2 f(w))^{-1} \nabla f(w), \nabla f(w) \rangle^{1/2}.
\]

We say that \( f \) is a **standard** s.c. function if \( M_f = 1 \). Let \( F \) be a standard s.c. function. We call it a s.c. barrier for the set \( \text{Dom} F \), if for all \( w \in \text{Dom} F \) we have:

\[
\sup_{u \in \mathbb{R}^n} \left[ 2 \langle \nabla F(w), u \rangle - \langle \nabla^2 F(w)u, u \rangle \right] \leq v.
\]

Note the difference between the domain of \( F \), \( \text{dom} F \), and the set for it is considered to be a barrier, \( \text{Dom} F \). For non-degenerate \( F \), the left-hand side could be replaced by \( \lambda_F^2(w) \). For equivalent definitions and more, see [Nesterov, 2018, Chapter 5].

### 4 Regression Algorithm

Our learning setting entails solving the following optimization problem: given the sample \((X_i, Y_i)_{i \in [n]}\), we wish to compute \( w \in [0, 1]^n \) that minimizes the empirical risk

\[
R_n(w) := \sum_{i=1}^n \left[ -Y_i \ln(w_i) - (1 - Y_i) \ln(1 - w_i) \right],
\]
subject to the truncation constraints \( \theta \leq w_i \leq 1 - \theta \) (the value of \( \theta \) will be determined in the sequel, see subsection 6.3; for now it is a fixed parameter), and the Lipschitz constraints \( |w_i - w_j| \leq L \rho(X_i, X_j) \), for all \( i, j \in [n] \).

We observe right away that our objective function is strictly convex and the feasible set is linearly constrained, hence the problem has a unique minimizer \( w^* \). The main result of this section is

**Theorem 4.1.** An \( \varepsilon \)-additive approximation to the problem stated above can be computed in time \( O \left( n^4 \ln \frac{2}{\varepsilon} \right) \).

Our algorithm relies on interior point methods, and is a close variant of the one presented in [Nesterov, 2018]. Throughout this section, we denote by the feasible set by \( Q \), the objective function by \( f_0 \), and the barrier function for the set \( Q \) by \( F \). We assume both \( f_0, F \) to be non-degenerate (in the sense that the Hessian is positive-definite) self-concordant functions, and in particular, \( F \) is a \( \nu \)-self-concordant barrier.

\( \beta, \gamma \) are constants to be specified later in this section. In our case, the objective is \( R_n(w) \), and \( F \) enforces the solution to be \( L \)-Lipschitz inside \( [\theta, 1 - \theta]^n \).

**Algorithm 1:** Path-following for Log-Likelihood

```
initialization: \( t = 0, k = 1 \);

while \( t_k < \frac{\beta(\beta + \sqrt{\nu})}{\varepsilon(1 - \beta)} \) do
    \( t_k = t_{k-1} + \frac{\gamma}{\|\nabla f_0(w_{k-1})\|^2_{t_{k-1}}} \);  \\
    \( w_k = w_{k-1} + \left[ t_k \nabla^2 f_0(w) + \nabla^2 F(w) \right]^{-1} (t_k \nabla f_0(w) + \nabla F(w)) \);  \\
    \( k = k + 1 \);
end
```

4.1 Interior point method and Logarithmic functions

In [Nesterov, 2018], the author defines the path-following scheme for linear functions, then generalizes it to non-linear functions by adding the objective as a constraint, thus minimizing the epigraph of the objective. Although we could utilize this technique,\(^1\) it requires adjustments to the LP framework, and additional auxiliary path-following iterations. Instead, we opt for minimizing the objective directly — an approach applicable to any self-concordant function. Additionally, this allows acceleration of the path-following scheme, as the step size is tied to the dual norm of a non-linear gradient.

**Consistency.** The path-following scheme is a succession of one-step Newton method iterations, where we gradually give more and more weight to the objective. In order to guarantee quadratic convergence, the condition \( \lambda_f(w) < \frac{1}{M_f} \) is required throughout the whole process: After every Newton step and increment in \( t \), the path-following parameter. Let denote our objective \( f_0(w), F(w) \) as the barrier. Then the path-following objective becomes

\[
f(w; t) = tf_0(w) + F(w),
\]

with self-concordant parameter, \( M_f(t) = \max \{M_{f_0}/\sqrt{t}, M_F\} \). In addition, recall the definitions of the primal and dual local norms (See technical background). We now extend these notations to include \( t \):

\[
\|u\|_{w,t} = \langle \nabla^2 f(w; t)u, u \rangle^{1/2} \\
\|u\|_{w,t}^* = \langle [\nabla^2 f(w; t)]^{-1} . u, u \rangle^{1/2}
\]

\(^1\)A barrier for epigraph of \(- \log(x)\) can be obtained, see [Nesterov, 2018, Theorem 5.3.5].
Further applying it to the definition of the local norm of the gradient,
\[ \lambda_{w,t} = \| \nabla f(w, t) \|_{w,t}^* = \langle (\nabla^2 f(w; t))^{-1} \nabla f(w; t), \nabla f(w; t) \rangle^{1/2}. \]

Note that the derivatives are taken only with respect to \( w \). Before we proceed to prove consistency of path-following for non-linear objective, we invoke a standard fact in positive semi-definite order to prove a lemma. Note that since \( f_0, F \) are non-degenerate, then so is \( f(w; t) \). Thus, \( \nabla^2 f(w; t) > 0 \) for all \( w \in \text{dom } f \).

The following is a standard fact [Horn and Johnson, 2012, Corollary 7.7.4(a)]:

**Lemma 4.1.** Let \( A, B \) be \( n \times n \) symmetric matrices. If \( 0 \preceq A \preceq B \) then
\[ A^{-1} \succeq B^{-1}. \]

Now let us apply it to the local norm.

**Lemma 4.2.** Let \( \nabla^2 f(w; t) > 0 \), then for all \( t \geq 0, \Delta t > 0 \) we have
\[ \| u \|_{w,t,\Delta t}^* \leq \| u \|_{w,t}^*. \]

**Proof:** Note that
\[ \nabla^2 f(w; t + \Delta t) \succeq \nabla^2 f(w; t). \]
Using Lemma 4.1:
\[ \| u \|_{w,t,\Delta t}^* = \langle (\nabla^2 f(w; t + \Delta t))^{-1} u, u \rangle^{1/2} \leq \langle (\nabla^2 f(w; t))^{-1} u, u \rangle^{1/2} = \| u \|_{w,t}^*. \]

The following argument closely follows [Nesterov, 2018, Lemma 5.2.2].

**Theorem 4.2.** Let \( t_+ = t + \frac{\gamma}{M_f(t)\| \nabla f(t) \|_{w,t}} \) and let the pair \( (w, t) \) satisfy:
\[ \| \nabla f(w; t) \|_{w,t}^* \leq \frac{\beta}{M_f(t)} \]
where \( \beta = \frac{\tau^2}{(1 - \tau)^2}, \quad \tau \leq \frac{1}{2}. \)

Then for \( \gamma \) satisfying
\[ |\gamma| \leq \tau - \frac{\tau^2}{(1 - \tau)^2}, \]
we have again \( \| \nabla f(w_+; t_+) \|_{w_+,t_+}^* \leq \frac{\beta}{M_f(t_+)} \).

**Proof:** First we apply Lemma 4.2 to switch between the norms:
\[ \| \nabla f(w_+,t_+) \|_{w_+,t_+}^* \leq \| \nabla f(w, t_+) \|_{w,t}^*. \]

Then
\[ \| \nabla f(w, t_+) \|_{w,t}^* \leq \| \nabla f(w, t_+) \|_{w,t}^* + \Delta t \| \nabla f(w) \|_{w,t}^* \leq \frac{\beta + \gamma}{M_f(t)} = \frac{\tau}{M_f(t)} \leq \frac{\tau}{M_f(t_+)}. \]
Using [Nesterov, 2018, Theorem 5.2.2] (i) we get:

\[ \| \nabla f(w_+; t_+) \|_{w_+, t_+}^* \leq \frac{M_f(t_+) \left( \| \nabla f(w, t_+) \|_{w, t_+} \right)^2}{\left( 1 - M_f(t_+) \| \nabla f(w, t_+) \|_{w, t_+} \right)^2} \leq \frac{\frac{M_f(t_+)}{(1 - \tau)^2}}{M_f(t_+)} = \tau. \]

□

Remark 4.1. We can assume \( M_f(t) = 1 \) from now on; the proof of the previous result shows that this incurs no loss of generality.

4.2 Runtime complexity

In order obtain runtime guarantees, we need to show that both the functional gap and local norm of objective gradient decrease with \( t \). These theorems are parallel to [Nesterov, 2018, Theorem 5.3.10, Lemma 5.3.2], respectively. Their proof can be found in the appendix.

Theorem 4.3. Let point \( w_t \) satisfy \( \| \nabla f(w_t; t) \|_{w_t, t}^* \leq \beta \). Then

\[ f_0(w_t) - f_0(w_{opt}) \leq \frac{1}{t} \left( v + \frac{\beta(\beta + \sqrt{v})}{1 - \beta} \right), \]

where

\[ w_{opt} = \arg\min_{w \in \text{dom } F} f(w). \]

Lemma 4.3. Let \( \| \nabla f(w; t) \|_{w_t, t}^* \leq \beta \), then

\[ \| \nabla f_0(w) \|_{w_t, t}^* \leq \frac{1}{t} (\beta + \sqrt{v} + \gamma). \]

We now proceed to the analytic complexity bound, which closely follows [Nesterov, 2018, Theorem 5.3.11]. The proof appears in the appendix.

Theorem 4.4. The maximum number of iterations of the above scheme is

\[ O \left( \sqrt{v} \ln \frac{v \| \nabla f(w_0) \|_{w_0, 0}^*}{\varepsilon} \right). \]

4.3 Runtime of Log-likelihood optimizer

The above states the number of path-following iterations. Now we’ll derive complete runtime analysis for our problem. First, Let us choose \( \tau \) so as to maximize our step in \( t \):

\[ \tau = 0.2291, \quad \gamma = 0.14, \quad \beta = 0.088. \]

Secondly, we construct a barrier for the domain of our problem. From this construction we obtain the barrier parameter, \( v = (n - 1)n \).

A quick observation reveals that the analytic center is trivial. The Lipschitz barrier is minimized when all coordinates are equal. Further setting them all to \( \frac{1}{2} \) also minimizes the box constraints. Thus, we can skip auxiliary path-following, setting \( w_0 = \frac{1}{2} \cdot 1_n \).
Additionally, it can be shown that:
\[ \| \nabla f(w_0) \|_{x_0,t_0}^n \leq \sqrt{n}. \]

A detailed derivation of these is presented in the Supplementary Material.

Finally, we’ll need to derive the arithmetical complexity of each iteration.

Each iteration involves two complexities: One is of the oracle, i.e. calculation of gradient and Hessian at current point, the other is calculation of the newton step. The derivatives calculation is dominated by the Lipschitz barrier gradient and hessian, where each requires \( O(n^2) \) operations. Calculating the next step in \( w \) (and in \( t \)) is dominated by the computation the inverse of \( \nabla^2 f(w;t) \). As this is a \( n \times n \) matrix, this involves \( O(n^3) \) operations. Thus, the arithmetical complexity of a single path-following iteration is \( O(n^2) \), for a total of \( O(n^4 \ln \frac{1}{\delta}) \).

### 4.4 Lipschitz extension

In this section, we show how to evaluate our hypothesis on a new point. Having computed an optimal hypothesis \( \hat{h} \) on the sample \( S \) via Algorithm 1, we wish to evaluate its prediction at a test point \( x \notin S \) via the Lipschitz extension technique. As this method is by now standard [von Luxburg and Bousquet, 2004, Gottlieb et al., 2017, Gottlieb et al., 2014], we present a brief sketch only. Formally, if \( S = \{x_1, \ldots, x_n\} \) and \( \hat{h} : S \to \mathbb{R} \), we wish to compute a value \( y = \tilde{h}(x) \) that minimizes \( \max_{i \in [n]} \left| \frac{y - \hat{h}(x_i)}{\rho(x, x_i)} \right| \). By the McShane-Whitney theorem [McShane, 1934, Whitney, 1934], the extension of \( \tilde{h} \) to the new point does not increase the Lipschitz constant of \( \hat{h} \), and so the risk bound in Theorem 6.1 applies.

The exact Lipschitz extension label \( y \) of \( x \notin S \) will always be determined by a pair of points \( x_i, x_j \in S \), one with label greater than \( y \) and one with a label less than \( y \), s.t. :

\[
L = \frac{\hat{h}(x_i) - y}{\rho(x, x_i)} = \frac{y - \hat{h}(x_j)}{\rho(x, x_j)} \geq \frac{|y - \hat{h}(x')|}{\rho(x, x')}, x' \in S
\]

Note that \( y \) cannot be increased or decreased without increasing the Lipschitz constant with respect to one of these points. Therefore, an exact Lipschitz extension may be computed in \( O(n^2) \) time in brute-force fashion, by enumerating all point pairs in \( S \), calculating the exact Lipschitz extension for \( x \) with respect to each pair alone, i.e.,

\[
y_{ij} = \frac{\hat{h}(x_j)\rho(x, x_i) + \hat{h}(x_i)\rho(x, x_j)}{\rho(x, x_i) + \rho(x, x_j)}
\]

and then select the one that achieves the highest Lipschitz constant.

### 5 Lower bound

The next theorem shows the necessity of truncation, at least when selecting hypotheses via Empirical Risk Minimization (ERM). We do this by demonstrating that minimizing empirical risk over untruncated classes (with predictions arbitrarily close to 0 or 1) leads to arbitrarily bad excess risk. Recall our loss function \( \ell \) defined in (1). For a fixed distribution \( \mu \) over \( \mathcal{X} \times \{0,1\} \), the expected risk of a hypothesis \( h : \mathcal{X} \to [0,1] \) is \( R(h) = \mathbb{E}_{(X,Y) \sim \mu}[\ell(Y,h(X))] \). The minimizer\(^2\) of the empirical risk is called Bayes-optimal and denoted by \( h^\ast \). If \( (X_i,Y_i)_{i \in [n]} \) is drawn from \( \mu^n \), it induces the empirical measure \( \mu_n \) and empirical risk \( R_n(h) = \mathbb{E}_{(X,Y) \sim \mu^n}[\ell(Y,h(X))] \); the empirical risk minimizer (whose existence and uniqueness were surmised above from convexity) is denoted by \( \hat{h}_n \). A given hypothesis class \( \mathcal{H} \subseteq [0,1]^\mathcal{X} \) induces the realizable setting if \( h^\ast \in \mathcal{H} \); otherwise, the setting is agnostic. Finally, we say that \( \mathcal{H} \) is \( \theta \)-truncated if \( \mathcal{H} \subseteq [\theta,1-\theta]^\mathcal{X} \).

\(^2\)Assuming a unique minimizer incurs no loss of generality.
Observation on risks: Because entropy of a Bernoulli random variable is bounded, the risk of the Bayes optimal is bounded by $\ln 2$. However, the loss on any data point $(x, y)$ is not bounded, and the risk of an arbitrary hypothesis is not bounded.

5.1 Necessity of truncation for the realizable case

The key point of the following example is that if we only observe samples of the form $(x, 0)$ but never $(x, 1)$, then empirical risk is minimized by choosing $h(x)$ as small as possible; but this could be a ruinous choice for expected risk. Truncation is a means of guarding against this.

**Theorem 5.1.** Suppose a hypothesis class $\mathcal{H}$ is not $e^{-O(n)}$-truncated. Then for any $\varepsilon > 0$ and large enough $n$, there exists a distribution where $R(\hat{h}_n) \geq R(h^*) + \varepsilon$ with probability at least $\frac{1}{2}$.

**Proof:** Given $\varepsilon > 0$ and large enough $n$, choose $h, x$ such that (without loss of generality) $h(x) \leq e^{-4\varepsilon n}$. This is possible because $\mathcal{H}$ is not $e^{-O(n)}$-truncated. Consider a distribution on $X = \{x\}$ with $h^*(x) = \frac{1}{2n}$.

By a union bound, with probability at least $\frac{1}{2}$, every example in the sample is of the form $(x, 0)$, and none is of the form $(x, 1)$. In this event, empirical risk of any hypothesis $h$ depends only on $h(x)$ and is monotonically decreasing in $h(x)$. So in this event, we have $\hat{h}_n(x) \leq e^{-4\varepsilon n}$, because in the worst case we have $\hat{h}_n = h$. But in this event, the excess risk of $\hat{h}_n$ is minimized when $\hat{h}_n(x)$ is closest to $h^*(x) = \frac{1}{2n}$. So in this event, letting $H(p)$ be the binary entropy function, we have

$$
= R(\hat{h}_n) - R(h^*) \\
\geq \left\lceil \frac{1}{2n} \ln e^{4\varepsilon n} + (1 - \frac{1}{2n}) \ln \frac{1}{1 - e^{4\varepsilon n}} \right\rceil - H(\frac{1}{2n}) \\
\geq 2\varepsilon - H(\frac{1}{2n}) \\
\geq \varepsilon \quad \text{(for large enough } n). \tag*{\Box}
$$

We note that in particular if $\mathcal{H}$ is not $e^{-n}$ truncated, then we can take $\varepsilon = 1$ in the above proof and obtain an impossibility result for all sample sizes $n \geq 1$.

5.2 Necessity of truncation for the agnostic case

Now we argue that agnostic learning is unlikely to be achievable without $e^{-O(\sqrt{n})}$-truncating the hypothesis classes. We use a simple family of examples where, with constant probability, ERM selects a hypothesis whose risk is worse than the optimal-in-class by a constant.

**Theorem 5.2.** There exist constants $\varepsilon, \delta > 0$ and input distribution $\mu$ such that, for any number of samples $n$, the following holds: there is a hypothesis class $\mathcal{H}$ of size two that is not $e^{-\sqrt{n}}$ truncated such that $\Pr[R(\hat{h}_n) \geq \min_{h \in \mathcal{H}} R(h) + \varepsilon] \geq \delta$.

**Proof:** Below, we will define the instance and family $\mathcal{H}$ of the form $\{h_1, h_2\}$. We then show in Claim 5.1 that, for all $n$, $\mathcal{H}$ has $R(h_2) \geq R(h_1) + \Omega(1)$. Finally, Claim 5.2 will show that $\Pr[\hat{h}_n = h_2] \geq \Omega(1)$.

It will be convenient here to take the base of the logarithm in (1) to be 2 rather than $e$. We consider a three-point space, $X = \{1, 2, 3\}$. The distribution $\mu$ on $X \times \{0, 1\}$ is completely uniform. In particular, $h^*(x) = 0.5$ for all $x \in X$.

Now define the hypothesis class $\mathcal{H}$, containing two hypotheses (we will pick $C$ based on $n$ later):
\begin{align*}
x &= 1 \quad x = 2 \quad x = 3 \\
h_1(x) &= \frac{1}{2} \quad \frac{1}{2} \quad 2^{-C} \\
h_2(x) &= \frac{1}{2} \quad 2^{-C} \quad \frac{1}{2}
\end{align*}

**Claim 5.1.** $R(h_2) - R(h_1) \geq 0.04$ for any $C > 0$.

**Proof:** The hypotheses are symmetric conditioned on $x \neq 1$. Conditioned on $x = 1$, which case occurs with probability $\frac{1}{3}$, the difference in expected loss is

\[
\left[ \frac{1}{2} \log(4) + \frac{1}{2} \log\left(\frac{3}{2}\right) \right] - \left[ \frac{1}{2} \log(2) + \frac{1}{2} \log(2) \right] = \frac{1}{2} \log\left(\frac{3}{2}\right).
\]

The difference in risks is $\frac{1}{6} \log\left(\frac{3}{2}\right) = 0.0479$. \hfill \Box

**Claim 5.2.** With $n$ examples, suppose $C > \sqrt[4]{n}$, implying that $\mathcal{H}$ is not $2^{-\sqrt[4]{n}}$-truncated. Then, with constant probability, the empirical risk of $h_2$ is smaller than that of $h_1$.

First we give a sketch, then the proof.

**Proof:** [Sketch] First, the difference in empirical risks due to samples where $X = 1$ is $O(n)$. Second, the difference due to samples where $X = 2$ or $X = 3$ is $\pm \Omega(n)$ with constant probability. So in total, with constant probability $h_1$ has larger empirical loss.

To see why there can be such a large difference in empirical loss due to samples where $X = 2$ or $X = 3$: when we obtain a sample where $X = 2$ or $X = 3$, with probability $\frac{1}{2}$ one of the hypotheses suffers a loss of $\log 2^C = C = \Omega(\sqrt[4]{n})$. With constant probability, this occurs $\Omega(\sqrt[4]{n})$ times more for $h_2$ than for $h_1$. In this case $h_2$ suffers an empirical loss on these samples that is larger by $\Omega(\sqrt[4]{n})\Omega(\sqrt[4]{n}) = \Omega(n)$. \hfill \Box

**Proof:** [Full] Write $\hat{R}(h_i)$ for the empirical loss of hypothesis $h_i$ on samples $(X,Y)$ where $X = x$. That is, $\hat{R}(h_i) = \sum_{j:x_j=x} L(h_i(x_j), y_j)$. We note $n \cdot R_n(h_i) = \hat{R}^1(h_i) + \hat{R}^2(h_i) + \hat{R}^3(h_i)$.

Now, let $N(j)$ be the number of examples where $X = j$ and $N(j,k)$ be the number where $X = j$ and $Y = k$. We calculate:

\[
\begin{align*}
\hat{R}^1(h_1) &= N(1), \\
\hat{R}^1(h_2) &= N(1,0) \log \frac{4}{3} + 2N(1,1) \\
&\leq 2N(1), \\
\hat{R}^2(h_1) &= N(2), \\
\hat{R}^2(h_2) &= N(2,0) \log \frac{1}{1-2^{-C}} + N(2,1)C, \\
\hat{R}^3(h_1) &= N(3,0) \log \frac{1}{1-2^{-C}} + N(3,1)C, \\
\hat{R}^3(h_2) &= N(3).
\end{align*}
\]

We compute $R_n(h_1) - R_n(h_2)$ by dividing the terms into two parts. First,

\[
\begin{align*}
\hat{R}^1(h_1) + \hat{R}^2(h_1) - \hat{R}^1(h_2) - \hat{R}^3(h_2) \\
&\geq N(1) + N(2) - 2N(1) - N(3) \\
&= N(2) - N(1) - N(3) \geq -n.
\end{align*}
\]

Second, let $\beta = \log \frac{1}{1-2^{-C}}$. Because $C \geq 1$, $\beta \leq 1$.

\[
\begin{align*}
\hat{R}^3(h_1) - \hat{R}^2(h_2) \\
&= \beta (N(3,0) - N(2,0)) + C (N(3,1) - N(2,1)) \\
&\geq -n + C (N(3,1) - N(2,1)).
\end{align*}
\]
In total, we get
\[ n \cdot R_n(h_1) - n \cdot R_n(h_2) \geq -2n + C \left( N(3, 1) - N(2, 1) \right). \]

It follows from Corollary C.1 that with constant probability, \( N(3, 1) - N(2, 1) > 2\sqrt{n} \). So with constant probability, \( n \cdot R_n(h_1) - n \cdot R_n(h_2) > -2n + \sqrt{n}(2\sqrt{n}) = 0 \). \( \square \)

5.3 Almost-matching upper bound for finite hypothesis classes

We observe that the above lower bound is tight, in a sense: We can agnostically learn, given a finite hypothesis class \( \mathcal{H} \), if it is \( e^{-o(\sqrt{n})} \)-truncated. This may be surprising, as with only \( n \) samples, it is in a sense not possible even to tell whether \( h^* \) is only \( \Omega(n) \) truncated (see Theorem 5.1). We sketch the idea here, again using base-2 loss.

Suppose \( H \) is \( 2^{-\theta} \)-truncated. The loss on any given data point is between zero and \( \log 2 = \theta \).

So the empirical loss \( R_n \) of a hypothesis, by Hoeffding’s inequality, satisfies
\[ \Pr \left( |R_n(h) - R(h)| \geq \varepsilon \right) \leq 2e^{-2n\varepsilon^2/\theta^2}. \]

Union-bounding over the finite hypothesis class, we obtain that with \( n \) samples, except with probability \( \delta \), we can obtain the hypothesis of optimal risk up to error at most
\[ \varepsilon = \theta \sqrt{\frac{\log \frac{2|\mathcal{H}|}{\delta}}{2n}}. \]

For \( \theta = o(\sqrt{n}/\log |\mathcal{H}|) \), this goes to zero by taking more and more samples \( n \).

6 Upper bound

The algorithm in Section 4 produces a hypothesis \( h \in \mathcal{H}_L \). This section is devoted to proving that with high probability, \( R(h, q) \) is not much greater than \( R_n(h, q) \).

**Theorem 6.1.** For \( L \geq 1 \) and every \( \delta > 0 \), we have that, with probability at least \( 1 - \delta \),
\[ R(h) - R_n(h) \leq O \left( \frac{1}{\theta} \left( \frac{L^d}{n} \right)^{\frac{1}{d+1}} \right) + 3 \ln \frac{1}{\theta} \sqrt{\frac{\ln(2/\delta)}{2n}} \]
holds uniformly over all \( L \)-Lipschitz \( [\theta, 1 - \theta] \)-valued hypothesis, where \( Z = (X_i, Y_i)_{i \in [n]} \) is the training sample.

**Remark.** Throughout the paper, we are treating the Lipschitz constant \( L \) of the hypothesis as known in advance. In practice, it would be chosen by cross-validation or Structural Risk Minimization [Shawe-Taylor et al., 1998]. Both techniques are standard, and we defer their detailed application to our case to the journal version.

6.1 Covering numbers for Lipschitz function classes

We begin by obtaining complexity estimates for Lipschitz functions in doubling spaces. We obtain simple and tight bounds by direct control over the covering numbers.

The following covering number lemma appears in [Gottlieb et al., 2017]; we state it here with slightly better constants:
Lemma 6.1. Let $\mathcal{F}_L$ be the collection of $L$-Lipschitz functions mapping the metric space $(X, \rho)$ to $[0, 1]$. Then the covering numbers of $\mathcal{F}_L$ may be estimated in terms of the covering numbers of $X$:

$$N(\varepsilon, \mathcal{F}_L, \|\cdot\|_\infty) \leq \left(\frac{3}{\varepsilon}\right)^{N(\varepsilon/4L, X, \rho)}.$$

Hence, for doubling spaces with $\text{diam}(X) = 1$,

$$\ln N(\varepsilon, \mathcal{F}_L, \|\cdot\|_\infty) \leq \left(\frac{8L}{\varepsilon}\right)^{\text{dim}(X)} \ln \left(\frac{3}{\varepsilon}\right).$$

See Appendix for proof of the above.

6.2 Rademacher complexities

The (empirical) Rademacher complexity [Bartlett, 2002] of a collection of functions $\mathcal{F}$ mapping some set $Z$ to $\mathbb{R}$ is defined, with respect to a sequence $Z = (Z_i)_{i\in[n]} \in Z^n$, by

$$\hat{R}_n(\mathcal{F}; Z) = \mathbb{E} \left[ \sup_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \sigma_i f(Z_i) \right],$$

where the expectation is over the $\sigma_i$, which are iid with $\mathbb{P}(\sigma_i = +1) = \mathbb{P}(\sigma_i = -1) = 1/2$.

To any collection $\mathcal{H}$ of hypotheses mapping $X$ to $[\tau, 1 - \tau]$, we associate the KL-loss class, whose members map $X \times \mathbb{R}$ to $\mathbb{R}$. The latter is denoted by $\mathcal{G}$ and defined to be

$$\mathcal{G} = \{g : (x, y) \mapsto -y \ln(h(x)) - (1 - y) \ln(1 - h(x))\}$$

where $h \in \mathcal{H}$.

We now move to prove the following variant of Theorem 3.3 in [Mohri, 2012]:

Theorem 6.2. For every $\delta > 0$, we have that, with probability at least $1 - \delta$,

$$R(h) \leq R_n(h) + 2\hat{R}_n(\mathcal{G}; Z) + 3 \ln \frac{1}{\theta} \sqrt{\frac{\ln(2/\delta)}{2n}},$$

holds uniformly over all $h \in \mathcal{H} = [\theta, 1 - \theta]^X$, where $Z = (X_i, Y_i)_{i\in[n]}$ is the training sample.

Proof: Let us Fix 2 samples $Z, Z'$ which differ by one point, and define the following function:

$$\Phi(Z) = \sup_{g \in \mathcal{G}} \left( \mathbb{E}[g] - \mathbb{E}_Z[g] \right)$$

Since the difference of suprema does not exceeds the suprema of the difference:

$$|\Phi(Z) - \Phi(Z')| \leq \frac{1}{n} \sup_{g \in \mathcal{G}} |g(z) - g(z')| =$$

$$\frac{1}{n} \sup_{h \in \mathcal{H}_C} |\frac{1}{n} \sum_{i=1}^{n} \sigma_i f(Z_i) - \frac{1}{n} \sum_{i=1}^{n} \sigma_i f(Z'_i)|.$$

As $y, y'$ takes values in $\{0, 1\}$, the above is equivalent to

$$\frac{1}{n} \sup_{h, h' \in [\theta, 1 - \theta]} \left\{ \ln \frac{h'}{h} \right\} \leq \frac{1}{n} \ln \frac{1 - \theta}{\theta} \leq \frac{1}{n} \ln \frac{1}{\theta}.$$
Due to symmetry we can bound $|\Phi(Z) - \Phi(Z')| \leq \frac{1}{n} \ln \frac{1}{\theta}$. Using McDiarmid’s inequality we get that with probability of $1 - \frac{\delta}{2}$:

$$
\phi(Z) \leq 2\mathcal{R}_n(\mathcal{G}) + \ln \frac{1}{\theta} \sqrt{\ln \frac{2}{2n}}.
$$

Where $\mathbb{E}_Z[\phi(Z)] = 2\mathcal{R}_n(\mathcal{G})$. Using similar arguments we can bound $|\widehat{\mathcal{R}}_n(\mathcal{G}; Z) - \widehat{\mathcal{R}}_n(\mathcal{G}; Z')| \leq \frac{1}{n} \ln \frac{1}{\theta}$. Using McDiarmid a second time, we get that with probability of $1 - \frac{\delta}{2}$:

$$
\mathcal{R}_n(\mathcal{G}) \leq \widehat{\mathcal{R}}_n(\mathcal{G}; Z) + \ln \frac{1}{\theta} \sqrt{\ln \frac{2}{2n}}.
$$

Using union bound we get that for any $h \in \mathcal{H}_L$, $\delta > 0$, the following holds:

$$
\mathbb{E}(g) \leq \frac{1}{n} \sum_{i=1}^{n} g(z_i) + 2\widehat{\mathcal{R}}_n(\mathcal{G}; Z) + 3 \ln \frac{1}{\theta} \sqrt{\ln \frac{2}{2n}}.
$$

As $\mathcal{H}$ is a truncated away from zero, it is easy to notice that $\mathcal{G}$ is $\frac{1}{\theta}$-Lipschitz. Using the following observation, we can apply Talagrand’s contraction lemma to connect the Rademacher complexities, of $\mathcal{H}$ and $\mathcal{G}$.

Given a fixed sample $Z$ as defined above, for each pair $(X_i, Y_i)$ every $g \in \mathcal{G}$ is either $\log h(X_i)$ or $\log \left(1 - h(X_i)\right)$, depending on $Y_i$. We get that both functions share the same Lipschitz constant of $\frac{1}{\theta}$. Thus let us replace $g(z_i)$ by $\phi_i(x)$, where the latter replaces the corresponding logarithmic function. Let us recall Talagrand’s contraction principle [Mohri, 2012, Lemma 5.7]:

**Lemma 6.2.** Let $\phi_1, ..., \phi_n$ be a $\frac{1}{\theta}$-Lipschitz function class from $\mathbb{R} \mapsto \mathbb{R}$. Then, for any hypothesis set $\mathcal{H}$ of real-valued functions and any sample $Z = (X_i)_{i=1}^{n}$, the following holds:

$$
\mathbb{E} \left[ \sup_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \sigma_i(\phi_i \circ h)(x_i) \right] \leq \frac{1}{\theta} \mathcal{R}_n(\mathcal{H}; Z).
$$

Equipped with the covering numbers estimate, we proceed to bound the Rademacher complexity of Lipschitz functions on doubling spaces.

**Theorem 6.3.** Let $\mathcal{F}_L$ be a collection of $L$-Lipschitz $[0,1]$-valued functions defined on a metric space $(\mathcal{X}, \rho)$ with diameter 1 and doubling dimension $d \geq 1$. Then

$$
\mathcal{R}_n(\mathcal{F}_L; Z) = O \left( \frac{L^{d+1}}{n^{d+1}} \right).
$$

See appendix for proof.

Combining Lemma 6.2 with Lemma 6.2 and Theorem 6.3, the generalization bound, Theorem 6.1 is immediate.

### 6.3 Choice of Truncation

The generalization bound Theorem 6.1 suggests an optimal truncation rate of $\theta = n^{-\frac{1}{d+2}}$. This is quite a bit more aggressive than the truncation rates of $\exp(-O(n))$ and $\exp(-O(\sqrt{n}))$ necessitated by the lower bounds in Section 5. Obtaining refined generalization bounds that allow for less aggressive truncation is an active research direction.
References

[Bartlett, 2002] Bartlett, M. (2002). Rademacher and gaussian complexities: Risk bounds and structural results. *Journal of Machine Learning Research*, 3:463–482.

[Choudhuri et al., 2007] Choudhuri, N., Ghosal, S., and Roy, A. (2007). Nonparametric binary regression using a gaussian process prior. *Statistical Methodology*, 4(2):227 – 243.

[Dubhashi and Ranjan, 1998] Dubhashi, D. and Ranjan, D. (1998). Balls and bins: a study in negative dependence. *Random Struct. Algorithms*, 13(2):99–124.

[Glavic, 2004] Glavic, W. (2004). Interior point methods: A survey, short survey of applications to power systems, and research opportunities.

[Gottlieb et al., 2014] Gottlieb, L., Kontorovich, A., and Krauthgamer, R. (2014). Efficient classification for metric data. *IEEE Transactions on Information Theory*, 60(9):5750–5759.

[Gottlieb et al., 2017] Gottlieb, L.-A., Kontorovich, A., and Krauthgamer, R. (2017). Efficient regression in metric spaces via approximate Lipschitz extension (extended abstract: SIMBAD 2013). *IEEE Transactions on Information Theory*, 63(8):4838–4849.

[Györfi et al., 2002] Györfi, L., Kohler, M., Krzyżak, A., and Walk, H. (2002). *A Distribution-Free Theory of Nonparametric Regression*. Springer New York.

[Hastie, 1983] Hastie, T. J. (1983). Non-parametric logistic regression. Technical Report SLAC-PUB-3160, Stanford Linear Accelerator Center and Department of Statistics, Stanford University.

[Horn and Johnson, 2012] Horn, R. A. and Johnson, C. R. (2012). *Matrix Analysis*. Cambridge University Press, USA, 2nd edition.

[Kim et al., 2020] Kim, Y., Carbonetto, P., Stephens, M., and Anitescu, M. (2020). A fast algorithm for maximum likelihood estimation of mixture proportions using sequential quadratic programming. *Journal of Computational and Graphical Statistics*, 29(2):261–273.

[Krauthgamer, 2004] Krauthgamer, L. (2004). Navigating nets: Simple algorithms for proximity search. *15th Annual ACM-SIAM Symposium on Discrete Algorithms*, pages 791–801.

[Lesaja, 2009] Lesaja, G. (2009). Introducing interior-point methods for introductory operations research courses and/or linear programming courses. *The Open Operational Research Journal*, 3(1):1–12.

[McShane, 1934] McShane, E. J. (1934). Extension of range of functions. *Bull. Amer. Math. Soc.*, 40(12):837–842.

[Mizera, 2014] Mizera, K. . (2014). Convex optimization, shape constraints, compound decisions, and empirical bayes rules. *Journal of the American Statistical Association*, 109:674–685.

[Mohri, 2012] Mohri, Rostamizadeh, T. (2012). Foundations of machine learning. | The MIT Press|.

[Nesterov, 2018] Nesterov, Y. (2018). *Lectures on Convex Optimization*. Springer Publishing Company, Incorporated, 2nd edition.

[Rasmussen and Williams, 2005] Rasmussen, C. E. and Williams, C. K. I. (2005). *Gaussian Processes for Machine Learning (Adaptive Computation and Machine Learning)*. The MIT Press.
[Shawe-Taylor et al., 1998] Shawe-Taylor, J., Bartlett, P. L., Williamson, R. C., and Anthony, M. (1998). Structural risk minimization over data-dependent hierarchies. *IEEE Transactions on Information Theory*, 44(5):1926–1940.

[Simonoff, 1996] Simonoff, J. S. (1996). *Smoothing Methods in Statistics*. Springer New York.

[Terlaky, 1995] Terlaky, V. (1995). Computing maximum likelihood estimators of convex density functions. *SIAM Journal on Scientific Computing*.

[Tsybakov, 2008] Tsybakov, A. B. (2008). *Introduction to Nonparametric Estimation*. Springer Publishing Company, Incorporated, 1st edition.

[Tsybakov, 2009] Tsybakov, A. B. (2009). *Introduction to Nonparametric Estimation*. Springer New York.

[von Luxburg and Bousquet, 2004] von Luxburg, U. and Bousquet, O. (2004). Distance-based classification with Lipschitz functions. *Journal of Machine Learning Research*, 5:669–695.

[Wasserman, 2006] Wasserman, L. (2006). *All of Nonparametric Statistics*. Springer New York.

[Whitney, 1934] Whitney, H. (1934). Analytic extensions of differentiable functions defined in closed sets. *Transactions of the American Mathematical Society*, 36(1):63–89.

[Young, 2012] Young, N. (2012). Reverse chernoff bound. Theoretical Computer Science Stack Exchange. URL:https://cstheory.stackexchange.com/q/14476 (version: 2012-11-26).

[Zhu and Hastie, 2002] Zhu, J. and Hastie, T. (2002). Kernel logistic regression and the import vector machine. In Dietterich, T. G., Becker, S., and Ghahramani, Z., editors, *Advances in Neural Information Processing Systems 14*, pages 1081–1088. MIT Press.
A Deferred proofs

A.1 Proof of Theorem 4.3

Proof: Let \( w_t^* \) be the minimizer of the path-following scheme for a given \( t \):

\[
w_t^* = \underset{w \in \text{dom } F}{\text{argmin}} \ f(w; t)
\]

Thus:

\[
\nabla f(w_t^*; t) = t\nabla f_0(w_t^*) + \nabla F(w_t^*) = 0.
\]

Additionally:

\[
\|\langle u, v \rangle \| \leq \|u\|_{w,t} \|v\|_{w,t}.
\]

We split the proof into 2 parts. Observe that

\[
f_0(w_t) - f_0(w_{opt}) = \frac{f_0(w_t) - f_0(w_t^*) + f_0(w_t^*) - f_0(w_{opt})}{(i)} + \frac{f_0(w_t^*) - f_0(w_t)}{(ii)}.
\]

(i) Since \( f_0 \) is self-concordant function, using [Nesterov, 2018, Theorem 5.1.8] we get:

\[
f_0(w_t^*) \geq f_0(w_t) + \langle \nabla f_0(w_t), w_t^* - w_t \rangle + \omega(\|w_t^* - w_t\|_{w,t}).
\]

As \( \omega(\tau) \geq 0 \forall \tau \geq 0 \), it can be dropped, leaving us with:

\[
f_0(w_t) - f_0(w_t^*) \leq -\langle \nabla f_0(w_t), w_t^* - w_t \rangle.
\]

Multiplying by \( t \) we get:

\[
t[f_0(w_t) - f_0(w_{opt})] \leq \langle -t\nabla f_0(w_t), w_t^* - w_t \rangle \leq \| -t\nabla f_0(w_t) \|_{w_t, t} \|w_t^* - w_t\|_{w_t, t} \leq \beta \frac{\beta}{1 - \beta}.
\]

Where the last transition is due the definition of self-concordant barrier alongside lemma 4.2, and [Nesterov, 2018, Theorem 5.2.1] with the definition of the auxiliary function \( \omega_t \).

(ii) Similarly, we’ve:

\[
f_0(w_t^*) - f_0(w_{opt}) \leq \langle -\nabla f_0(w_t^*), w_{opt} - w_t^* \rangle.
\]

Multiplying by \( t \) we get

\[
t[f_0(w_t^*) - f_0(w_{opt})] \leq \langle -t\nabla f_0(w_t^*), w_{opt} - w_t^* \rangle = \langle \nabla F(w_t^*), w_{opt} - w_t^* \rangle \leq v.
\]

The last transition is due to [Nesterov, 2018, Theorem 5.3.7].

A.2 Proof of Lemma 4.3

Proof:

\[
t\|\nabla f_0(w)\|^{*}_{w,t} = \|(t - \Delta t) + \Delta t\|\nabla f_0(w)\|^{*}_{w,t} \leq \|\nabla f(w; t - \Delta t) - \nabla F(w)\|^{*}_{w,t-\Delta t} + \Delta t\|\nabla f_0(w)\|^{*}_{w,t-\Delta t} \leq \beta + \sqrt{v} + \gamma.
\]
A.3 Proof of Theorem 4.4

Proof: Due to Lemma 4.3:

\[
\begin{align*}
        t_k &= t_{k-1} \left( 1 + \frac{\gamma}{t_{k-1} \| \nabla f(w_{k-1}) \|_{w_{k-1},t_{k-1}}} \right) = \\
        t_1 \prod_{i=1}^{k-1} \left( 1 + \frac{\gamma}{t_i \| \nabla f(w_i) \|_{w_i,t_i}} \right) \geq \\
        \frac{\| \nabla f(w_0) \|_{w_0,0}^*}{(1 + \frac{\gamma}{\gamma + \beta + \sqrt{\beta}})^{k-1}}.
\end{align*}
\]

After some manipulations we get that \( \forall k \geq 1: \)

\[
\ln \left( \frac{t_k \| \nabla f(w_0) \|_{w_0,t_0}^*}{\gamma} \right) \geq (k-1) - \frac{1}{\gamma + \beta + \sqrt{\beta}} + 1 \geq k,
\]

where we used \( \ln(1 + x) \geq \frac{x}{2}. \)

A.4 Proof of Lemma 6.1

Proof: Fix a covering of \( \mathcal{X} \) consisting of \(|N| = N(\varepsilon', \mathcal{X}, \rho)\) balls \( \{U_1, \ldots, U_{|N|}\} \) of radius \( \varepsilon' = \varepsilon/4L \) and choose \(|N|\) points \( N = \{x_i \in U_i\}_{i=1}^{|N|} \). We will construct an \( \varepsilon \)-cover \( \hat{F} = \{\hat{f}_1, \ldots, \hat{f}_{|\hat{F}|}\} \) as follows. At every point \( x_i \in N \), we choose \( \hat{f}(x_i) \) to be of the following form, while maintaining \( \|\hat{f}\|_{1,\text{lip}} \leq 2L: \)

\[
2kL\varepsilon', k = 0, 1, 2, \ldots
\]

Construct a \( 2L \)-Lipschitz extension for \( \hat{f} \) from \( N \) to all over \( \mathcal{X} \) (such an extension always exists, [McShane, 1934, Whitney, 1934]). We claim that every \( f \in \mathcal{F}_L \) is close to some \( \hat{f} \in \hat{F} \), in the sense that \( \|f - \hat{f}\|_\infty \leq \varepsilon \). Indeed, every point \( x \in \mathcal{X} \) is \( \varepsilon' \)-close to some point \( x_N \in N \), and since \( f \) is \( L \)-Lipschitz and \( \hat{f} \) is \( 2L \)-Lipschitz,

\[
|f(x) - \hat{f}(x)| \leq L \cdot \rho(x, x_N) + L\varepsilon' + 2L \cdot \rho(x, x_N) = 4L\varepsilon' = \varepsilon.
\]

It is easy to verify that \( |\hat{F}| \leq (3/\varepsilon)^{|N|} \), since by construction, the functions \( \hat{f} \) are determined by their values on \( N \). This provides a covering of \( \mathcal{F}_L \) using \( |\hat{F}| \) balls of radius \( \varepsilon \).

The bound for doubling spaces follows immediately by applying the so-called doubling property (see for example [Krauthgamer, 2004]) and the diameter bound, to obtain

\[
N(\varepsilon', \mathcal{X}, \rho) \leq \frac{2^{d\dim(\mathcal{X})}}{\varepsilon'} = \left(\frac{8L}{\varepsilon}\right)^{d\dim(\mathcal{X})}.
\]

\( \square \)
A.5 Proof of Theorem 6.3

**Proof:** Recalling that for norms induced by probability measures, we have \( \|f\|_2 \leq \|f\|_\infty \), we can substitute the estimate in Lemma 6.1 to get:

\[
\hat{R}_n(\mathcal{F}_L; Z) \leq \inf_{\alpha \geq 0} \left( 4\alpha + 12 \int_{\alpha}^{\infty} \sqrt{\frac{\ln N(t, \mathcal{F}_L, \|\cdot\|_\infty)}{n}} \, dt \right) \leq \inf_{\alpha \geq 0} \left( 4\alpha + 12 \int_{\alpha}^{\infty} \sqrt{\frac{(2\pi)^d}{n} \ln (\frac{2}{\alpha})} \, dt \right) \leq \inf_{\alpha \geq 0} \left( 4\alpha + 12 \int_{\alpha}^{\infty} \sqrt{\frac{(2\pi)^d}{n} \ln (\frac{2}{\alpha})} \, dt \right) = \inf_{\alpha \geq 0} \left( 4\alpha + 24(8L)^{d/2} \sqrt{n} \right)
\]

where \( K = \frac{24(8L)^{d/2}}{\sqrt{n}} + \frac{2}{d - 1} \).

The optimal value is obtained by deriving:

\[
\alpha^* = \left( \frac{K(d-1)}{8} \right)^{\frac{2}{d+1}}
\]

Assuming \( d \geq 1 \), by assigning \( \alpha^* \) and taking \( C \) to infinity we get:

\[
4 \left( \frac{K(d-1)}{8} \right)^{\frac{2}{d+1}} + K \left( \frac{K(d-1)}{8} \right)^{\frac{2}{d+1}} \leq 3.
\]

Noticing that

\[
\left( \frac{d-1}{8} \right)^{\frac{1}{d+1}} \leq 3,
\]

We have

\[
4 \left( \frac{K(d-1)}{8} \right)^{\frac{2}{d+1}} + K \left( \frac{K(d-1)}{8} \right)^{\frac{2}{d+1}} \leq 3 \left( 4K^{\frac{2}{d+1}} + K^{\frac{2}{d+1}} \right) \leq 15 K^{\frac{2}{d+1}}.
\]

Further assigning \( K \) we get the stated bound with a constant \( c = 2520 \). \( \square \)

B Construction of the barrier

As all constraints are linear, the construction of the self-concordant Barrier is simple. Though the box constraints are actually redundant (The objective can serve as a barrier for itself), since the Hessian of the Lipschitz constraint is singular, we’ve to maintain the box boundary to avoid it.

Additionally, the objective serves as the box barrier (except for the case that all samples are 1 or 0, which is trivial), so only the Lipschitz constraints are considered.

Let \( L \) be a symmetric \( n \times n \) matrix, where \( L_{ij} = Ld_T(X_i, X_j) \).

Let \( \zeta(i, j) = (w_i - w_j + L_{ij}) \).

\[
F(w) = F_Q(w) + F_L(w), \quad F_Q(w) = -\sum_{i=1}^{n} [\ln (w_i) + \ln (1 - w_i)], \quad F_L(w) = -\sum_{1 \leq i < j \leq n} [\ln \zeta(j,i) + \ln \zeta(i,j)].
\]
The gradient and hessian are:

\[ \frac{\partial F_Q(w)}{\partial w_i} = -w_i^{-1} + (1 - w_i)^{-1}, \quad \frac{\partial F_L(w)}{\partial w_i} = \sum_{j \neq i} [\zeta(j, i)^{-1} - \zeta(i, j)^{-1}] \]
\[ \frac{\partial^2 F_Q(w)}{\partial w_i \partial w_j} = w_i^{-2} + (1 - w_i)^{-2}, \quad \frac{\partial^2 F_L(w)}{\partial w_i \partial w_j} = -\zeta(j, i)^{-2} - \zeta(i, j)^{-2} \]
\[ \frac{\partial^2 F_Q(w)}{\partial w_i \partial w_j} = 0, \quad \frac{\partial^2 F_L(w)}{\partial w_i \partial w_j} = \sum_{j \neq i} [\zeta(j, i)^{-2} + \zeta(i, j)^{-2}] = -\sum_{j \neq i} \frac{\partial^2 F_L(w)}{\partial w_i \partial w_j}. \]

The barrier parameter is dominated by the Lipschitz constraints, thus we can set

\[ v = (n - 1)n = O(n^2). \]

In order to calculate \( \|\nabla f_0(w_0)\|_{w_0,0}^* \), first note that since \( t = 0 \):

\[ \nabla^2 f(w_0) = \nabla^2 F(w_0) \geq \nabla^2 f_0(w_0). \]

Since we choose \( w_0 \) s.t. \( w_0(i) = 1/2, i \in [n] \), then \( \nabla^2 F_L(w_0) = 0 \). Thus, it can be calculated directly:

\[ \|\nabla f_0(w_0)\|_{w_0,0}^* = \frac{\|\nabla^2 f_0(w_0)\|^{-1}}{\|\nabla f_0(w_0)\|^2} = \sqrt{\sum_{i=1}^{n} \left( \frac{1}{2} \right)^{-1}} = \sqrt{n} \]

\section{Anti-concentration lemmas}

The following “Reverse Chernoff bound” is due to [Young, 2012]:

\textbf{Lemma C.1.} Suppose that \( X \sim \text{Binomial}(n, p) \), and \( 0 < \varepsilon, p \leq 1/2 \) satisfy \( \varepsilon^2 np \geq 3 \). Then

\[ \Pr(X \leq (1 - \varepsilon)pn) \geq \exp(-9\varepsilon^2 pn), \]
\[ \Pr(X \geq (1 + \varepsilon)pn) \geq \exp(-9\varepsilon^2 pn). \]

\textbf{Corollary C.1.} There is a universal constant \( c > 0 \) for which the following holds. Let \( \mu \) be the uniform distribution on the 6-point set \( X = \{1, \ldots, 6\} \) and let \( \mu_n \) be its empirical realization induced by an iid sample of size \( n \). Define the random variables \( X = n\mu_n(\{1\}) \) and \( X' = n\mu_n(\{2\}) \); each is distributed according to Binomial\((n, p)\), where \( p = 1/6 \) \((X, X' \text{ are not independent})\). For \( n \geq 324 \), we have

\[ \Pr(X - X' > 2\sqrt{n}) \geq c. \]

\textbf{Proof:} We choose \( \varepsilon = 1.5/(p\sqrt{n}) \leq 1/2 \) and verify that \( \varepsilon^2 np = 2.25/p = 13.5 > 3 \), so the conditions of Lemma C.1 hold. Now \( \varepsilon np = 1.5\sqrt{n} \) and we have that \( \Pr(X \geq np + 1.5\sqrt{n}) \geq \exp(-20.25/p) = e^{-121.5} \) and \( \Pr(X' \leq np - 1.5\sqrt{n}) \geq e^{-121.5} \). By inclusion of events,

\[ \Pr(X - X' > 2\sqrt{n}) \geq \Pr(X \geq np + 1.5\sqrt{n}, X' \leq np - 1.5\sqrt{n}). \]

Observe that \( X, X' \) are negatively associated [Dubhashi and Ranjan, 1998], which implies that \( \Pr(X \geq s, X' \leq t) \geq \Pr(X \geq s)\Pr(X' \leq t) \) for all \( s, t \). It follows that

\[ \Pr(X - X' > 2\sqrt{n}) \geq \Pr(X \geq np + 1.5\sqrt{n}) \cdot \Pr(X' \leq np - 1.5\sqrt{n}) \geq e^{-243} =: c > 0. \]

\[ \Box \]