

Optimization for Machine Learning

Reading group, Fall 2017

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1 Introduction

Speaker: Patrick Rebeschini, 12/10/2017.

Many problems in statistics and machine learning can be formulated as the problem of computing

$$x^* \in \arg \min_{x \in \mathcal{X}} r(x), \quad (1)$$

where $r(x) := \mathbf{E} \ell(x^T \Phi(W), Y)$, given only data in the form of m i.i.d. labeled samples $(W_1, Y_1), \dots, (W_m, Y_m) \sim (W, Y) \in \mathcal{W} \times \mathcal{Y}$, i.e., without knowledge of the distribution of (W, Y) (in particular, without knowledge of the function r that we want to minimize!). Here, the function $\Phi : \mathcal{W} \rightarrow \mathbb{R}^n$ (known) is a feature map, the function $x \in \mathcal{X} \subseteq \mathbb{R}^n \rightarrow x^T \Phi(W)$ is the linear predictor for the label Y (\mathcal{X} is known), the function $\ell : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ (known) is a loss function characterizing the penalty in committing a wrong prediction, and $r(x)$ is the *test cost* or *expected risk* associated to the parameter x . In this setting, one wants to find x^* that yields the best linear predictor over unseen data using the data in the training set, relying on the assumption that the unseen data share the same (unknown) distribution of observed samples.

In binary classification, one has $\mathcal{Y} = \{-1, 1\}$ and loss functions are typically of the form $\ell(z, y) = \varphi(-zy)$. A few examples are:

- Zero-One loss (a.k.a. the true loss): $\varphi(u) = \mathbf{1}_{u \geq 0}$.
- Exponential loss: $\varphi(u) = \exp(u)$.
- Hinge loss: $\varphi(u) = \max\{0, 1 + u\}$ (giving SVM).
- Logistic loss: $\varphi(u) = \log_2(1 + \exp(u))$.

In regression, one has $\mathcal{Y} = \mathbb{R}$, and the typical loss is:

- Least-squares loss: $\ell(u, y) = (u - y)^2$.

Perhaps the most intuitive paradigm for solving problem (1) is the *empirical risk minimization*, that is, the idea to minimize the *training cost* or *empirical risk*:

$$R(x) := \frac{1}{m} \sum_{i=1}^m R_i(x),$$

where $R_i(x) := \ell(x^T \Phi(W_i), Y_i)$. This approach is motivated by the fact that for each $x \in \mathcal{X}$ the law of large number gives $r(x) \approx R(x)$ so that one might expect that $x^* \approx X^*$, where $X^* \in \arg \min_{x \in \mathcal{X}} R(x)$. This intuition can be made precise, and Proposition 1 below shows that the estimation error $r(X^*) - r(x^*) \geq 0$ can be controlled by suprema of random processes.

Proposition 1. *We have*

$$r(X^*) - r(x^*) \leq \sup_{x \in \mathcal{X}} (r(x) - R(x)) + \sup_{x \in \mathcal{X}} (R(x) - r(x)).$$

Proof. By adding and subtracting terms, we get

$$r(X^*) - r(x^*) = r(X^*) - R(X^*) + R(X^*) - R(x^*) + R(x^*) - r(x^*).$$

As X^* is a minimizer of R , we have $R(X^*) - R(x^*) \leq 0$. The proof follows by taking the supremum over $x \in \mathcal{X}$. \square

This analysis assumes that one can actually compute an exact minimizer X^* for the training cost R . With a finite amount of computational resources available, however, typically one can only compute an approximate minimizer. Let $\hat{X}_t \in \mathcal{X}$ denote an approximate solution to $\arg \min_{x \in \mathcal{X}} R(x)$ that is computed after t iterations of a given algorithmic procedure. Proceeding as above we have the following result.

Proposition 2. *We have*

$$r(\hat{X}_t) - r(x^*) \leq \underbrace{\sup_{x \in \mathcal{X}} (r(x) - R(x)) + \sup_{x \in \mathcal{X}} (R(x) - r(x))}_{\text{STATISTICS}} + \underbrace{R(\hat{X}_t) - R(X^*)}_{\text{OPTIMIZATION}}. \quad (2)$$

Proof. By adding and subtracting terms, we get

$$r(\hat{X}_t) - r(x^*) = r(\hat{X}_t) - R(\hat{X}_t) + R(\hat{X}_t) - R(X^*) + R(X^*) - R(x^*) + R(x^*) - r(x^*).$$

As X^* is a minimizer of R , we have $R(X^*) - R(x^*) \leq 0$. The proof follows by taking the supremum over $x \in \mathcal{X}$. \square

The problem is now to estimate how close the expected risk of the approximate empirical risk minimizer $r(\hat{X}_t)$ is to the minimal expected risk $r(x^*)$ in terms of the number of training samples m , the dimension of the feature map n , the number of iterates t for the optimization routine, and the other parameters that define the model at hand (for example, the radius of the parameter set \mathcal{X} , properties of the loss function ℓ , and of the feature map Φ). To this end, as Proposition 2 shows, we need to control two terms: the *STATISTICS* term $\sup_{x \in \mathcal{X}} (r(x) - R(x)) + \sup_{x \in \mathcal{X}} (R(x) - r(x))$ and the *OPTIMIZATION* term $R(\hat{X}_t) - R(X^*)$.

In the first part of the reading group we will focus on algorithms that can be used to approximately minimize the empirical risk and hence control the *OPTIMIZATION* term in (2), making various assumptions for the loss function ℓ and the parameter space \mathcal{X} , starting from the fruitful assumption of convexity.¹ Along with convexity, we state some of the main properties that a generic function f can have that are used to assess the quality of algorithms to minimize f . Here we assume that f is differentiable, but analogous notions can be defined for non-differentiable functions using the notion of subgradients. We also mention in brackets equivalent (local) definitions, which apart from L -Lipschitz hold when f is twice-differentiable.

- Convexity: $f(x) - f(y) \leq \nabla f(x)^T (x - y)$ for any $x, y \in \mathbb{R}^n$ ($\nabla^2 f(x) \succcurlyeq 0$ for any $x \in \mathbb{R}^n$).
- L -Lipschitz: $|f(x) - f(y)| \leq L \|x - y\|_2$ for any $x, y \in \mathbb{R}^n$ ($\|\nabla f(x)\|_2 \leq L$ for any $x \in \mathbb{R}^n$).
- β -Smoothness: $\|\nabla f(x) - \nabla f(y)\|_2 \leq \beta \|x - y\|_2$ for any $x, y \in \mathbb{R}^n$ ($\nabla^2 f(x) \preccurlyeq \beta I$ for any $x \in \mathbb{R}^n$).
- α -Strong convexity: $f(x) - f(y) \leq \nabla f(x)^T (x - y) - \frac{\alpha}{2} \|x - y\|_2^2$ for any $x, y \in \mathbb{R}^n$ ($\nabla^2 f(x) \succcurlyeq \alpha I$ for any $x \in \mathbb{R}^n$).

Going back to the losses defined above, it is easy to check that the following holds:

- Exponential loss: $\varphi(u) = \exp(u)$: Lipschitz NO, Smooth NO, strongly-convex NO.
- Hinge loss: $\varphi(u) = \max\{0, 1 + u\}$: Lipschitz YES, Smooth NO, strongly-convex NO.
- Logistic loss: $\varphi(u) = \log_2(1 + \exp(u))$: Lipschitz YES, Smooth YES, strongly-convex NO.
- Least-squares loss: $\ell(u, y) = (u - y)^2$: Lipschitz NO, Smooth YES, strongly-convex YES.

¹convexity is only needed to perform the analysis of the algorithms that we introduce, but it is not needed to run the algorithms themselves; in fact, in practice the algorithms that we define are run also on non-convex problems.

Note that as far as the empirical risk minimization goes, what we care about are the (almost sure) properties of the function $x \in \mathcal{X} \rightarrow R(x) := \frac{1}{m} \sum_{i=1}^m R_i(x) = \frac{1}{m} \sum_{i=1}^m \ell(x^T \Phi(W_i), Y_i)$. In particular, if \mathcal{X} is bounded, we can restrict the definitions above to hold on a bounded set. For instance, we could define L -Lipschitz as the property: $|f(x) - f(y)| \leq L\|x - y\|_2$ for any $x, y \in \mathbb{R}^n$ such that $\|x\|_2, \|y\|_2 \leq c$ ($\|\nabla f(x)\|_2 \leq L$ for any $x \in \mathbb{R}^n$ such that $\|x\|_2 \leq c$). Assuming boundedness provides extra flexibility, allowing one to directly use these properties in setting where otherwise they would not apply (take the exponential loss, for instance).

Even if we assume boundedness of \mathcal{X} , assuming that the empirical risk R is strongly convex is typically a strong assumption. In fact, note that for any $x \in \mathcal{X}$ (that is, regardless of the properties of \mathcal{X}) the Hessian

$$\nabla^2 R(x) = \frac{1}{m} \sum_{i=1}^m \frac{\partial^2}{\partial z^2} \ell(x^T \Phi(W_i), Y_i) \Phi(W_i) \Phi(W_i)^T \in \mathbb{R}^{n \times n}$$

is not invertible if $m < n$, being a sum of $m < n$ rank-1 matrices. So in this case $x \rightarrow \nabla^2 R(x)$ can not be strongly convex. In applications where $m \geq n$, the empirical covariance can be invertible, but it is typically the case that the strong convexity parameter α is very small, of order $1/m$, effectively $\alpha \approx 0$ (or close to machine precision) for applications involving large datasets. For this reason, in this reading group we will only focus on results about Lipschitz and smooth functions, which are more natural assumptions for the empirical risk R , as we now show.

First, note that if we assume that ℓ is L_{loss} -Lipschitz in the first coordinate, namely, $z \rightarrow \ell(z, y)$ is L_{loss} -Lipschitz for any $y \in \mathcal{Y}$, and that the feature map Φ is bounded in ℓ_2 , namely, $\|\Phi\|_2 \leq G$, then R is GL_{loss} -Lipschitz:

$$|R(x) - R(y)| \leq \frac{1}{m} \sum_{i=1}^m |\ell(x^T \Phi(W_i), Y_i) - \ell(y^T \Phi(W_i), Y_i)| \leq \frac{L_{\text{loss}}}{m} \sum_{i=1}^m \|(x - y)^T \Phi(W_i)\|_2 \leq GL_{\text{loss}} \|x - y\|_2,$$

where for the last inequality we used Cauchy-Schwarz. Second, note that if we assume that ℓ is β_{loss} -Lipschitz in the first coordinate, namely, $z \rightarrow \ell(z, y)$ is β_{loss} -Lipschitz for any $y \in \mathcal{Y}$, and that $\|\Phi\|_2 \leq G$, then R is $G^2\beta_{\text{loss}}$ -smooth:

$$\begin{aligned} \|\nabla R(x) - \nabla R(y)\|_2 &\leq \frac{1}{m} \sum_{i=1}^m \left\| \left(\frac{\partial}{\partial z} \ell(x^T \Phi(W_i), Y_i) - \frac{\partial}{\partial z} \ell(y^T \Phi(W_i), Y_i) \right) \Phi(W_i) \right\|_2 \\ &\leq \frac{1}{m} \sum_{i=1}^m \beta_{\text{loss}} |(x - y)^T \Phi(W_i)| \|\Phi(W_i)\|_2 \leq \beta_{\text{loss}} G^2 \|x - y\|_2. \end{aligned}$$

While this is a reading group on optimization, before we embark on the adventure of minimizing the empirical risk and bound the *OPTIMIZATION* term in (2), we should try to develop some basic understanding of what to expect from the behavior of the *STATISTICS* term as well. This understanding will give us insights on the type of precision that we should strive for to control the *OPTIMIZATION* term. To this end, we now give a brief detour on statistical learning theory and derive an explicit bound in the case when the loss function ℓ is Lipschitz (no assumption on convexity is made for this result), the feature map is bounded, and also the parameter space \mathcal{X} is bounded. While in this reading group we do not plan to prove other results such as the one that we present in the next section, nevertheless the proof is instructive and relies on classical machinery of concentration inequalities and Rademacher complexity.

1.1 Statistical learning theory

Statistical learning theory focuses on understanding how the estimation error $r(X^*) - r(x^*)$ converges to zero as a function of the sample size m , the loss function ℓ , the parameter space \mathcal{X} , and possibly some properties of the distribution of $\Phi(W)$ and Y (recall that the distribution themselves are not known). We will prove the following result, following the arguments as presented in [2].

Proposition 3. *If $z \rightarrow \ell(z, y)$ is L_{loss} -Lipschitz for any $y \in \mathcal{Y}$, $\|\Phi(W)\|_2 \leq G$ a.s., and $\sup_{x \in \mathcal{X}} \|x\|_2 \leq B$, then with probability at least $1 - \delta$ we have*

$$\text{STATISTICS} = \sup_{x \in \mathcal{X}} (r(x) - R(x)) + \sup_{x \in \mathcal{X}} (R(x) - r(x)) \leq 2 \frac{\ell_0 + GL_{\text{loss}}B}{\sqrt{m}} \left(4 + \sqrt{2 \log \frac{1}{\delta}} \right),$$

where $\ell_0 := \sup_{y \in \mathcal{Y}} |\ell(0, y)|$.

The quality of the bound in Proposition 3 is typical in statistical learning theory. In particular, it is typically the case that the *slow* rate $O(1/\sqrt{m})$ can not be improved, unless other assumptions are taken into consideration that allow to prove a *fast* rate $O(1/m)$. These upper bounds suggest² that we only need to approximate the *OPTIMIZATION* term up to precision $O(1/\sqrt{m})$ (resp. $O(1/m)$).

The next part of this section is devoted to proving Proposition 3. To this end, we need to bound suprema of a random processes. Henceforth, let us consider the following quantity (analogously, we can look at the symmetric quantity):

$$h(Z_1, \dots, Z_m) := \sup_{x \in \mathcal{X}} (r(x) - R(x)) = \sup_{x \in \mathcal{X}} \left(r(x) - \frac{1}{m} \sum_{i=1}^m R_i(x) \right), \quad (3)$$

where we use the notation $Z_i := (W_i, Y_i)$. A classical way to bound this quantity is by using concentration inequalities, which are tools in probability theory to bound the deviation of a function of many i.i.d. random variables to its mean. One of the classical concentration inequalities is the Bounded Difference, of which we now state a simple version.

Proposition 4 (Bounded Difference Inequality). *Let $Z_1, \dots, Z_m \in \mathcal{Z}$ be m i.i.d. random variables, and let $h : \mathcal{Z}^m \rightarrow \mathbb{R}$ be a function satisfying, for every $k \in \{1, \dots, m\}$ and for all $z_1, \dots, z_m, z'_k \in \mathcal{Z}$:*

$$|h(z_1, \dots, z_{k-1}, z_k, z_{k+1}, \dots, z_m) - h(z_1, \dots, z_{k-1}, z'_k, z_{k+1}, \dots, z_m)| \leq c.$$

Then,

$$\mathbf{P}(h(Z_1, \dots, Z_m) \geq \mathbf{E}h(Z_1, \dots, Z_m) + t) \leq \exp \left(- \frac{2t^2}{mc^2} \right),$$

or, equivalently, with probability at least $1 - \delta$ we have

$$h(Z_1, \dots, Z_m) \leq \mathbf{E}h(Z_1, \dots, Z_m) + c \sqrt{\frac{m}{2} \log \frac{1}{\delta}}.$$

To apply the Bounded Difference inequality to the function h defined in (3), we need to find c that satisfy the assumption of Proposition 4. The next proposition shows how to do this under the assumption of Proposition 3.

Proposition 5. *Let h be the function defined in (3) and consider the same assumption of Proposition 3. Then, $c \in \mathbb{R}$ satisfying the requirement of the Bounded Difference inequality is given by*

$$c = \frac{2}{m} \left(\sup_{y \in \mathcal{Y}} |\ell(0, y)| + GL_{\text{loss}}B \right).$$

²Caveats are in order: after all the result in (2) is only an upper-bound, and it is often the case that in practice one does not know the constants sitting in front of the error bounds that one can prove for both the *OPTIMIZATION* term and the *STATISTICS* term, i.e., the constants G, L, R in our case.

Proof. Fix $k \in \{1, \dots, m\}$ and let $z = (z_1, \dots, z_{k-1}, z_k, z_{k+1}, \dots, z_m)$ and $z' = (z_1, \dots, z_{k-1}, z'_k, z_{k+1}, \dots, z_m)$. Then,

$$|h(z) - h(z')| = \left| \sup_{x \in \mathcal{X}} \left(r(x) - \frac{1}{m} \sum_{i=1}^m R_i^z(x) \right) - \sup_{x \in \mathcal{X}} \left(r(x) - \frac{1}{m} \sum_{i=1}^m R_i^{z'}(x) \right) \right|,$$

where $R_i^z(x) := \ell(x^T \Phi(w_i), y_i)$. If $h(z) - h(z') \geq 0$ and we let $\tilde{x} \in \mathcal{X}$ be the maximizer of $\sup_{x \in \mathcal{X}} (r(x) - \frac{1}{m} \sum_{i=1}^m R_i^z(x))$ (note that the supremum is attained by the Extreme Value Theorem), we have

$$\begin{aligned} h(z) - h(z') &= \left(r(\tilde{x}) - \frac{1}{m} \sum_{i=1}^m R_i^z(\tilde{x}) \right) - \sup_{x \in \mathcal{X}} \left(r(x) - \frac{1}{m} \sum_{i=1}^m R_i^{z'}(x) \right) \\ &\leq \left(r(\tilde{x}) - \frac{1}{m} \sum_{i=1}^m R_i^z(\tilde{x}) \right) - \left(r(\tilde{x}) - \frac{1}{m} \sum_{i=1}^m R_i^{z'}(\tilde{x}) \right) \\ &= \frac{1}{m} (R_k^z(\tilde{x}) - R_k^{z'}(\tilde{x})) \leq \frac{2}{m} \sup_{x \in \mathcal{X}, z \in \mathcal{Z}} |R_k^z(x)|. \end{aligned}$$

Proceeding analogously in the case $h(z) - h(z') \leq 0$, we finally find

$$|h(z) - h(z')| \leq \frac{2}{m} \sup_{x \in \mathcal{X}, z \in \mathcal{Z}} |R_k^z(x)| = \frac{2}{m} \sup_{x \in \mathcal{X}, w \in \mathcal{W}, y \in \mathcal{Y}} |\ell(x^T \Phi(w), y)|.$$

Using, that $z \rightarrow \ell(z, y)$ is L_{loss} -Lipschitz for any $y \in \mathcal{Y}$ and Cauchy-Schwarz we get

$$|\ell(x^T \Phi(w), y)| \leq |\ell(0, y)| + |\ell(x^T \Phi(w), y) - \ell(0, y)| \leq |\ell(0, y)| + L_{\text{loss}} \|x^T \Phi(w)\|_2 \leq |\ell(0, y)| + L_{\text{loss}} \|x\|_2 \|\Phi(w)\|_2,$$

which, upon using $\|\Phi(W)\|_2 \leq G$ a.s. and $\sup_{x \in \mathcal{X}} \|x\|_2 \leq B$ yields

$$|\ell(x^T \Phi(w), y)| \leq |\ell(0, y)| + GL_{\text{loss}} B,$$

so that

$$|h(z) - h(z')| \leq \frac{2}{m} \left(\sup_{y \in \mathcal{Y}} |\ell(0, y)| + GL_{\text{loss}} B \right).$$

□

The bounded-difference inequality tells us that in order to control $h(Z_1, \dots, Z_m)$ we need to control the expectation $\mathbf{E}[h(Z_1, \dots, Z_m)]$. The following is a classical way of doing so, based on the Rademacher complexity.

Proposition 6. *We have*

$$\mathbf{E} \sup_{x \in \mathcal{X}} \left(r(x) - \frac{1}{m} \sum_{i=1}^m R_i(x) \right) \leq 2\mathcal{R},$$

where \mathcal{R} is the Rademacher complexity defined as

$$\mathcal{R} := \mathbf{E} \sup_{x \in \mathcal{X}} \frac{1}{m} \sum_{i=1}^m \varepsilon_i R_i(x),$$

with $\varepsilon_1, \dots, \varepsilon_n$ i.i.d. Rademacher random variables uniform in $\{-1, 1\}$, independent of Z_1, \dots, Z_n .

Proof. The proof uses the standard machinery of symmetrization. Let $\mathcal{D}' := \{Z'_1, \dots, Z'_m\}$ be an independent copy of the data $\mathcal{D} := \{Z_1, \dots, Z_m\}$. Using that $r(x) = \mathbf{E}R'_i(x) = \mathbf{E}[R'_i(x)|\mathcal{D}]$, we have

$$\begin{aligned}
\mathbf{E} \sup_{x \in \mathcal{X}} \left(r(x) - \frac{1}{m} \sum_{i=1}^m R_i(x) \right) &= \mathbf{E} \sup_{x \in \mathcal{X}} \frac{1}{m} \sum_{i=1}^m \mathbf{E}[R'_i(x) - R_i(x) | \mathcal{D}] \\
&\leq \mathbf{E} \mathbf{E} \left[\sup_{x \in \mathcal{X}} \frac{1}{m} \sum_{i=1}^m (R'_i(x) - R_i(x)) \middle| \mathcal{D} \right] \\
&= \mathbf{E} \sup_{x \in \mathcal{X}} \frac{1}{m} \sum_{i=1}^m (R'_i(x) - R_i(x)) \\
&= \mathbf{E} \sup_{x \in \mathcal{X}} \frac{1}{m} \sum_{i=1}^m \varepsilon_i (R'_i(x) - R_i(x)) \quad \text{by symmetrization} \\
&= 2\mathbf{E} \sup_{x \in \mathcal{X}} \frac{1}{m} \sum_{i=1}^m \varepsilon_i R_i(x).
\end{aligned}$$

□

We are left with bounding the Rademacher complexity.

Proposition 7. *Under the assumption of Proposition 3, we have*

$$\mathcal{R} \leq \frac{2GL_{\text{loss}}B}{\sqrt{m}}.$$

Proof. Note that there are two independent sources of randomness in the definition of \mathcal{R} . One comes from the Rademacher random variables $\varepsilon_1, \dots, \varepsilon_m$, the other comes from the data $\mathcal{D} := (Z_1, \dots, Z_m)$ itself. By the tower property we can isolate the effect of the Rademacher random variables and work conditionally on \mathcal{D} . That is,

$$\mathcal{R} = \mathbf{E} \mathbf{E} \left[\sup_{x \in \mathcal{X}} \frac{1}{m} \sum_{i=1}^m \varepsilon_i R_i(x) \middle| \mathcal{D} \right].$$

If for each $i \in \{1, \dots, m\}$ we define the functions $\varphi_i(u) := \ell(u, Y_i) - \ell(0, Y_i)$, we have

$$\begin{aligned}
\mathbf{E} \left[\sup_{x \in \mathcal{X}} \frac{1}{m} \sum_{i=1}^m \varepsilon_i R_i(x) \middle| \mathcal{D} \right] &= \mathbf{E} \left[\sup_{x \in \mathcal{X}} \frac{1}{m} \sum_{i=1}^m \varepsilon_i [R_i(0) + R_i(x) - R_i(0)] \middle| \mathcal{D} \right] \\
&\leq \mathbf{E} \left[\frac{1}{m} \sum_{i=1}^m \varepsilon_i R_i(0) \middle| \mathcal{D} \right] + \mathbf{E} \left[\sup_{x \in \mathcal{X}} \frac{1}{m} \sum_{i=1}^m \varepsilon_i [\ell(x^T \Phi(W_i), Y_i) - \ell(0, Y_i)] \middle| \mathcal{D} \right] \\
&= \frac{1}{m} \sum_{i=1}^m \mathbf{E}[\varepsilon_i | \mathcal{D}] R_i(0) + \mathbf{E} \left[\sup_{x \in \mathcal{X}} \frac{1}{m} \sum_{i=1}^m \varepsilon_i \varphi_i(x^T \Phi(W_i)) \middle| \mathcal{D} \right] \\
&= \mathbf{E} \left[\sup_{x \in \mathcal{X}} \frac{1}{m} \sum_{i=1}^m \varepsilon_i \varphi_i(x^T \Phi(W_i)) \middle| \mathcal{D} \right],
\end{aligned}$$

where for the last equality we used that by the independence between $\varepsilon_1, \dots, \varepsilon_m$ and \mathcal{D} we have $\mathbf{E}[\varepsilon_i | \mathcal{D}] = \mathbf{E}\varepsilon_i = 0$. As the function $z \rightarrow \ell(z, y)$ is L_{loss} -Lipschitz for any $y \in \mathcal{Y}$, also each function φ_i is L_{loss} -Lipschitz. By the

contraction property of Rademacher complexities (indeed, one of the reason why this notion of complexity is convenient to use), we have

$$\mathbf{E} \left[\sup_{x \in \mathcal{X}} \frac{1}{m} \sum_{i=1}^m \varepsilon_i \varphi_i(x^T \Phi(W_i)) \middle| \mathcal{D} \right] \leq 2L_{\text{loss}} \mathbf{E} \left[\sup_{x \in \mathcal{X}} \frac{1}{m} \sum_{i=1}^m \varepsilon_i x^T \Phi(W_i) \middle| \mathcal{D} \right].$$

Hence, using that $\sup_{x \in \mathcal{X}} \|x\|_2 \leq B$

$$\begin{aligned} \mathcal{R} &\leq 2L_{\text{loss}} \mathbf{E} \sup_{x \in \mathcal{X}} \frac{1}{m} \sum_{i=1}^m \varepsilon_i x^T \Phi(W_i) \\ &\leq 2L_{\text{loss}} \mathbf{E} \sup_{x \in \mathcal{X}} \|x\|_2 \left\| \frac{1}{m} \sum_{i=1}^m \varepsilon_i \Phi(W_i) \right\|_2 \quad \text{by Cauchy-Schwarz} \\ &\leq 2L_{\text{loss}} B \mathbf{E} \sqrt{\left\| \frac{1}{m} \sum_{i=1}^m \varepsilon_i \Phi(W_i) \right\|_2^2} \leq 2L_{\text{loss}} B \sqrt{\mathbf{E} \left\| \frac{1}{m} \sum_{i=1}^m \varepsilon_i \Phi(W_i) \right\|_2^2} \quad \text{by Jensen's inequality} \\ &= \frac{2L_{\text{loss}} B}{m} \sqrt{\mathbf{E} \sum_{j=1}^n \left(\sum_{i=1}^m \varepsilon_i \Phi(W_i)_j \right)^2} = \frac{2L_{\text{loss}} B}{m} \sqrt{\mathbf{E} \sum_{j=1}^n \sum_{i=1}^m (\varepsilon_i \Phi(W_i)_j)^2} \quad \text{by the independence of the } \varepsilon\text{'s} \\ &= \frac{2L_{\text{loss}} B}{m} \sqrt{\mathbf{E} \sum_{i=1}^m \varepsilon_i^2 \|\Phi(W_i)\|_2^2} \leq \frac{2GL_{\text{loss}} B}{\sqrt{m}} \quad \text{as } \|\Phi(W)\|_2 \leq G \text{ a.s.} \end{aligned}$$

□

The proof of Proposition 3 follows by putting everything together, namely, Proposition 4, Proposition 5, Proposition 6, and Proposition 7, noting that the bounds in high probability that we have obtained hold for *both* $\sup_{x \in \mathcal{X}} (r(x) - R(x))$ and $\sup_{x \in \mathcal{X}} (R(x) - r(x))$. Here are the details.

Proof of Proposition 3. Using, respectively, Proposition 4 and Proposition 6, we have that with probability at least $1 - \delta$ the following holds:

$$\sup_{x \in \mathcal{X}} (r(x) - R(x)) \leq \mathbf{E} \left[\sup_{x \in \mathcal{X}} (r(x) - R(x)) \right] + c \sqrt{\frac{m}{2} \log \frac{1}{\delta}} \leq 2\mathcal{R} + c \sqrt{\frac{m}{2} \log \frac{1}{\delta}},$$

where $c = \frac{2}{m}(\ell_0 + GL_{\text{loss}}B)$ by Proposition 5. Plugging in the bound for \mathcal{R} in Proposition 7, we get

$$\mathbb{P} \left(\sup_{x \in \mathcal{X}} (r(x) - R(x)) \leq c \right) \geq 1 - \delta,$$

where $c := 2(\ell_0 + GL_{\text{loss}}B)(4 + \sqrt{2 \log(1/\delta)})/\sqrt{m}$. As the bounds we have derived holds also for $\sup_{x \in \mathcal{X}} (R(x) - r(x))$, we have

$$\mathbb{P} \left(\sup_{x \in \mathcal{X}} (r(x) - R(x)) + \sup_{x \in \mathcal{X}} (R(x) - r(x)) \leq 2c \right) \geq \mathbb{P} \left(\left\{ \sup_{x \in \mathcal{X}} (r(x) - R(x)) \leq c \right\} \cap \left\{ \sup_{x \in \mathcal{X}} (R(x) - r(x)) \leq c \right\} \right) \geq 1 - \delta.$$

□

1.2 Plan for the rest of the term

Given the analysis of the previous section, we can now describe the plan for the reading group this term. While we motivated our interest in optimization techniques by looking at the classical setting of supervised machine learning and empirical risk minimization, only in Week 8 (hopefully!) we will see how to develop specialized algorithms to minimize R (that is, algorithms that can take advantage of the specific structure of R). In fact, most of our time will be devoted to reviewing classical algorithms to optimize a *general* convex function f over a convex set \mathcal{X} , namely, to solve:

$$\begin{aligned} & \text{minimize} && f(x) \\ & \text{subject to} && x \in \mathcal{X}. \end{aligned}$$

Below is the current plan of what we aim to cover, along with references to the corresponding literature.

IMPORTANT NOTE FOR SPEAKERS.

The results that are quoted in bold are the ones we will be focusing on. When presenting your section and typing up notes, focus only on covering these results, along with introducing the quantities/proofs that are needed. You might comment on the other results if you have time, or just to give an overview of the bigger picture. In other words, instead of trying to cover as much as possible content-wise, try to cover as little as possible with as much explanation as possible (pictures, intuition, etc.).

As we move along in the reading group, the plan below might change. Please make sure that you have the latest version of these lecture notes before you prepare your section.

Week 2: Convexity. Black-box model. Projected gradient descent methods.

Readings: Parts of Chapter 1 and Chapter 3 in [3]. Details are below.

We introduce convexity, and some of its basic properties, such as the existence of subgradients (**Proposition 1.1 in [3]**) and the first order optimality condition (**Proposition 1.3 in [3]**).

We introduce the black-box model of computation, where we assume that the constraint set $\mathcal{X} \subseteq \mathbb{R}^n$ is known and the objective function f is unknown but can be accessed through queries to first order oracles: given $x \in \mathcal{X}$, a first order oracle yields back a subgradient of f at x .

We study how the different assumptions of L -Lipschitz, β -Smoothness, and α -Strong convexity, lead to different convergence rates for projected subgradient descent methods. Upon different conditions, different projected subgradient descent methods achieve the following rates:

	L -Lipschitz	β -smooth
Convex	$O(BL/\sqrt{t})$	$O(B^2\beta/t)$
α -strongly convex	$O(L^2/(\alpha t))$	$O(B^2e^{-t\alpha/\beta})$

where B is the radius of the Euclidean ball that contains \mathcal{X} , namely, $\sup_{x \in \mathcal{X}} \|x\|_2 \leq B$. As we discuss earlier, for applications in machine learning the assumption of α -strong convexity is typically too strong. This is why we only prove the rates for the convex case, both for L -Lipschitz and for β -Smooth. For completeness, here is where to find all the results mentioned above:

- Convex & L -Lipschitz: $O(BL/\sqrt{t})$ (**Theorem 3.2 in [3]**).
- Convex & β -Smoothness: $O(B^2\beta/t)$ (**Theorem 3.7 and in [3]**).
- α -Strong convexity & L -Lipschitz: $O(L^2/(\alpha t))$ (Theorem 3.9 and in [3]).
- α -Strong convexity & β -Smoothness: $O(B^2 \exp(-t\alpha/\beta))$ (Theorem 3.10 and in [3]).

These results are sometimes called *dimension-free*, since as presented the rates do not depend explicitly on the ambient dimension n . However, the dependence on the dimension enters implicit in the constants: note that B is the radius of the constraint set $\mathcal{X} \subseteq \mathbb{R}^n$, and that the parameters L , α , and β , are defined in terms of the Euclidean norm in \mathbb{R}^n . The terminology dimension-free is used in [3] to differentiate the rates achieved by subgradient descent methods from the rates obtained by ellipsoid methods (Chapter 2 in [3]), which we will not cover in this reading group.

We can also phrase these results in terms of *oracle complexity*, namely, the number of queries to the oracle that are *sufficient* to find an ε -approximate minima of a convex function:

	L -Lipschitz	β -smooth
Convex	$O(B^2 L^2 / \varepsilon^2)$	$O(B^2 \beta / \varepsilon)$
α -strongly convex	$O(L^2 / (\alpha \varepsilon))$	$O((\beta / \alpha) \log(B^2 / \varepsilon))$

Remark 1. To conclude, let us go back to our motivating example of minimizing the empirical risk function $R(x) = \frac{1}{m} \sum_{i=1}^m \ell(x^T \Phi(W_i), Y_i)$. Under the assumptions of Proposition 3, R is GL_{loss} -Lipschitz (see Section 1). Assuming that the loss function ℓ is convex, the subgradient descent method then yields:

$$\text{OPTIMIZATION} := R(\hat{X}_t) - R(X^*) \leq \frac{GL_{\text{loss}} B}{\sqrt{t}}.$$

Here the constants are explicit, and they match the ones in Proposition 3 for the STATISTICS term. In particular, following the rationale of optimizing the OPTIMIZATION term in (2) up to the accuracy given by the STATISTICS term in (2), one finds that it suffices to run the algorithm for $t \sim m$ number of steps.

Week 3: Lower bounds for oracle complexity.

Readings: Parts of Chapter 3 in [3]. Details are below.

We see that within the first order oracle model one can prove lower-bounds for the amount of calls to the oracle that are *needed* to achieve a certain accuracy ε . In the non-smooth case we show that the rates achieved by subgradient descent methods, i.e., $O(BL/\sqrt{t})$ for convex functions and $O(L^2/(\alpha t))$ for α -strongly convex functions, can not be improved (**Theorem 3.13 in [3]; we will only cover the proof of the first statement for convex L -Lipschitz functions**). On the other hand, in the smooth case we prove oracle-complexity lower bounds that are better than the ones achieved by subgradient methods, namely, $O(D^2 \beta / t^2)$ for smooth functions (**Theorem 3.14 in [3]**) and $O(D^2 \exp(-t \sqrt{\alpha/\beta}))$ for smooth and strongly convex functions (Theorem 3.15 in [3]), where D is the diameter of \mathcal{X} , i.e., $D := \max_{x,y \in \mathcal{X}} \|x - y\|_2$. To recap, the optimal rates are:

	L -Lipschitz	β -smooth
Convex	$O(BL/\sqrt{t})$	$O(D^2 \beta / t^2)$
α -strongly convex	$O(L^2/(\alpha t))$	$O(D^2 e^{-t \sqrt{\alpha/\beta}})$

Week 4: Application: Boosting.

Reading: Parts of Part II, Section 1.4 and Part II, Section 2.2 in [4]. Details are below.

We apply the projected subgradient descent algorithm to solve an important example in machine learning: Boosting. For a given loss function φ (recall, $\ell(z, y) = \varphi(-zy)$ in classification), ℓ_1 -boosting can be written as the problem:

$$\begin{aligned} & \text{minimize} && r(x) = \mathbf{E} \varphi(-Y x^T \Phi(W)) \\ & \text{subject to} && x \in \Delta_m, \end{aligned}$$

where $\Delta_m := \{x \in [0, 1]^m : \sum_{k=1}^m x_k = 1\}$ is the m -dimensional probability simplex. Here the feature map $\Phi : \mathcal{W} \rightarrow \{-1, 1\}^n$ encodes the prediction of the n base classifiers on the given data point it is applied to, and $x^T \Phi$ is a linear combination of these classifiers. Following the error decomposition in Proposition 2, we show (**Part II, Section 1.4 in [4]**) that in this case the *STATISTICS* term is $O(\log(n)/\sqrt{m})$, which only grows logarithmically with the number of base classifiers n . This is a nice feature in applications where n is very large. Hence, one would hope to be able to design an algorithmic procedure that only uses $\log(n)$ calls to the oracle in order to match the accuracy of the *STATISTICAL* term when finding a solution to the empirical risk minimization problem:

$$\begin{aligned} \text{minimize} \quad & R(x) = \frac{1}{m} \sum_{i=1}^m \varphi(-Y_i x^T \Phi(W_i)) \\ \text{subject to} \quad & x \in \Delta_m. \end{aligned}$$

We show that if ϕ is L -Lipschitz, then the empirical risk minimizer R is $L\sqrt{n}$ -Lipschitz, so that projected subgradient descent yields a rate $O(L\sqrt{n}/t)$ (**Part II, Section 2.3.3 in [4]**). Imposing the condition $L\sqrt{n}/t \lesssim \log(n)/\sqrt{m}$, we find that $t \gtrsim L^2 nm / \log(n)^2$, which does *not* scale logarithmically with n as we hoped for. Boosting is one example where one would like to apply subgradient descent methods on a non-Euclidean space, in particular a ℓ_1 space, but these methods are not suited for this type of problems as they are really designed for Euclidean geometry. Note, in fact, that all the definitions we gave for L -Lipschitz, β -smoothness, α -strong convexity are expressed in terms of the Euclidean norm $\|\cdot\|_2$. This motivates the design of a new class of algorithms that can adapt to the geometry of the problem at hand, as we will see next.

Week 5: Non-Euclidean setting: mirror descent.

Readings: Section 4.1, 4.2, and 4.3 in [3]. Details are below.

We introduce the mirror descent algorithm and show that this algorithm adapts also to non-Euclidean geometries. We say that f is L -Lipschitz in some norm $\|\cdot\|$ if $|f(x) - f(y)| \leq L\|x - y\|$ for any $x, y \in \mathbb{R}^n$. We show that for such convex functions mirror descent yields rates that scale like $O(LB/\sqrt{t})$ (**Theorem 4.2 in [3]**). This allows mirror descent to achieve a rate $O(\sqrt{\log n}/t)$ in the example of boosting, where one wants to minimize a function with subgradient bounded in the ℓ_∞ -norm over the probability simplex (**Section 4.3 in [3]**), in contrast to the rate $O(\sqrt{n}/t)$ achieved by subgradient descent, as shown last time. We also show that in the case of the Euclidean norm, the algorithm is equivalent to projected subgradient descent.

Week 6: Acceleration by coupling gradient descent and mirror descent.

Readings: [1].

We show that mirror descent can be coupled with gradient descent to yield an *accelerated* algorithm that can achieve the lower bound for smooth functions that we proved in Week 3. The acceleration technique is linear coupling, from the paper [1].

Week 7: Non-Euclidean setting: Frank-Wolfe.

Readings: Section 3.3 in [3]. Details are below.

In many applications, the computational bottleneck in gradient descent methods is given by the projection step on the constraint set \mathcal{X} . To address this issue, we study the Frank-Wolfe algorithm (a.k.a. conditional gradient descent), which replaces the projection step with a linear optimization over \mathcal{X} , which in some cases can be a much simpler problem. For smooth objective functions, the Frank-Wolfe algorithm achieves rate $O(B^2\beta/t)$ (**Theorem**

3.8 in [3]). While this rare is slow and it does not match the oracle complexity lower bound $O(D^2\beta/t^2)$, the saving in the computational complexity makes this algorithm convenient in some applications. Other advantages of this algorithm over gradient descent methods is that this algorithm can apply to smoothness in any norm (f is β -smooth in some norm $\|\cdot\|$ if $\|\nabla f(x) - \nabla f(y)\|_* \leq \beta\|x - y\|$ for any $x, y \in \mathbb{R}^n$, where the dual norm $\|\cdot\|_*$ is defined as $\|g\|_* = \sup_{x \in \mathbb{R}^n: \|x\| \leq 1} g^T x$), and that the algorithm computes sparse iterates. We will discuss a concrete application where these benefits are substantial, the least square regression with structured sparsity (**in Section 3.3 in [3]**).

Week 8: Stochastic oracle model.

Readings: Section 6.1, 6.2, and 6.3 in [3].

The first order oracle model that we have investigated so far had allowed us to produce a complete theory of convex optimization, in the sense that for various classes of convex functions we can design algorithms with an *oracle complexity* that matches the lower bounds. However, the black-box model does not tell us anything about the *computational complexity*, namely, the number of elementary computations that an algorithm needs to do to solve the problem (indeed, to address this question we should “open” the black-box). Going back to the original problem in machine learning that we set to solve, as described in Section 1, we note that the first order oracle model is too general for our needs, and that there might be computational savings to be gained in working with a model of computation that is more fined-tuned to our problem. This consideration motivates us to consider the *stochastic* first order oracle model, where for any point $x \in \mathcal{X}$ the oracle gives back an unbiased estimator of the gradient at x . Within this framework, two approaches have attracted a lot of attention lately, due to the computational savings they yield.

Multiple passes over the data. Within the setting of empirical risk minimization, one notices that we know the *global* structure of the function we want to minimize, namely, $R = \frac{1}{m} \sum_{i=1}^m R_i$. Hence, for instance, given $x \in \mathcal{X}$ we can have access to $\nabla R_i(x)$ for a specific $i \in \{1, \dots, m\}$, which is something that is not allowed in the oracle model previously discussed where only access to $\nabla R(x)$ is granted. Note that computing $\nabla R(x)$ costs $O(m)$ operations as R is the sum of m terms, while computing $\nabla R_i(x)$ costs $O(1)$.

Single pass over the data. The empirical risk minimization approach described in Section 1 has allowed us to break the original problem we care about, namely, problem (1), into a *STATISTICAL* component and an *OPTIMIZATION* component, see Proposition 2. We show that within the stochastic oracle model there is a way to directly address problem (1) and yield a bound for $r(\hat{X}_t) - r(x^*)$, *combining* both statistics and optimization. Recall that we do not know the function r as we assume that we do not know the distribution of the random variables W and Y ; as a consequence, we also do not know the gradient of r , so we can not minimize r within the classical first order oracle model. On the other hand, we can treat the $\nabla R_i(x)$ ’s as unbiased estimators of ∇r .

2 Convexity. Black-box model. Projected gradient descent methods.

Speaker: Anthony Caterini, 19/10/2017.

We want to focus first on introducing the notion of convexity, which will admit some very nice properties for optimization. In particular, convex functions always have subgradients, and any local minimum is also a global minimum. We will also introduce projected subgradient descent methods and prove convergence rates in the cases where f is convex and either L -Lipschitz continuous or β -smooth. In these two cases, the essence of the method is the same, although the particulars are slightly different.

The methods in this section relate to controlling the *OPTIMIZATION* term in empirical risk minimization. We note that although the empirical risk R may not be convex, we can still run the algorithms that we discuss to find local optima.

Note that in this section, we rely heavily on [3], although the extension of projected gradient descent to time-varying step sizes comes from [4, Lecture 11, Page 5].

2.1 Convexity

We begin by recalling the definition of a convex function and convex set.

Definition 1 (Convex function and set). *A function $f : \mathcal{X} \subset \mathbb{R}^n \rightarrow \mathbb{R}$ is convex if, for all $(x, y, \gamma) \in \mathcal{X} \times \mathcal{X} \times [0, 1]$,*

$$f((1 - \gamma)x + \gamma y) \leq (1 - \gamma)f(x) + \gamma f(y).$$

In other words, f always lies below its chords. Similarly, a set $\mathcal{X} \subset \mathbb{R}^n$ is convex if, for all $(x, y, \gamma) \in \mathcal{X} \times \mathcal{X} \times [0, 1]$,

$$(1 - \gamma)x + \gamma y \in \mathcal{X}.$$

In other words, \mathcal{X} contains all of its line segments.

2.1.1 Existence of subgradients

We will also define the notion of a subgradient – useful when f is not differentiable – and show that a convex function always admits subgradients. This will be important when we introduce the projected subgradient method, as we will not assume differentiability of f . We will instead assume that f is convex, and that we have access to a *first order oracle* that can give us a subgradient of f at each point.

Definition 2 (Subgradient). *Let $\mathcal{X} \subset \mathbb{R}^n$ and $f : \mathcal{X} \rightarrow \mathbb{R}$. Then, $g \in \mathbb{R}^n$ is a subgradient of f at $x \in \mathcal{X}$ if, for any $y \in \mathcal{X}$, one has*

$$f(x) - f(y) \leq g^T(x - y).$$

The set of subgradients of f at x is denoted $\partial f(x)$.

Note that we can rewrite the above inequality as $f(y) \geq f(x) + g^T(y - x)$. Thus, each subgradient defines a plane that supports f . Also notice the set of subgradients at a point at which f is non-differentiable can be infinite. Conversely, we will see that, for convex and differentiable functions, the standard gradient is also a subgradient. We first mention the supporting hyperplane theorem and the definition of the epigraph before showing this.

Theorem 1 (Supporting Hyperplane Theorem). *Let \mathcal{X} be a convex set, and $x_0 \in \partial \mathcal{X}$ (the boundary of \mathcal{X}). Then, there exists $w \in \mathbb{R}^n$, $w \neq 0$, such that*

$$\forall x \in \mathcal{X}, w^T x \geq w^T x_0.$$

Definition 3 (Epigraph). *The epigraph of a function $f : \mathcal{X} \rightarrow \mathbb{R}$ is*

$$\text{epi}(f) = \{(x, t) \in \mathcal{X} \times \mathbb{R} : t \geq f(x)\}.$$

Also, a function is convex if and only if its epigraph is convex.

Proposition 8 (Existence of subgradients). *Let \mathcal{X} be convex and $f : \mathcal{X} \rightarrow \mathbb{R}$. If $\forall x \in \mathcal{X}, \partial f(x) \neq \emptyset$, then f is convex. Conversely, if f is convex, then for any $x \in \text{int}(\mathcal{X})$, $\partial f(x) \neq \emptyset$. Furthermore, if f is convex and differentiable at x , then $\nabla f(x) \in \partial f(x)$.*

Proof. For the first claim, let $g \in \partial f((1 - \gamma)x + \gamma y)$, for any $x, y \in \mathcal{X}$ and $\gamma \in [0, 1]$. Then,

$$f((1 - \gamma)x + \gamma y) \leq f(x) + \gamma g^T(y - x), \quad (4)$$

$$f((1 - \gamma)x + \gamma y) \leq f(y) + (1 - \gamma)g^T(x - y). \quad (5)$$

Then, adding $(1 - \gamma) \cdot (4)$ with $\gamma \cdot (5)$ clearly shows that f is a convex function.

Now let us suppose that f is convex. Let $x \in \mathcal{X}$. Clearly, $(x, f(x)) \in \partial \text{epi}(f)$, and $\text{epi}(f)$ is a convex set. Thus, by the Supporting Hyperplane Theorem, there exists $(a, b) \in \mathbb{R}^n \times \mathbb{R}$, $(a, b) \neq 0$, such that for all $(y, t) \in \text{epi}(f)$,

$$a^T x + b f(x) \geq a^T y + b t. \quad (6)$$

By allowing $t \rightarrow \infty$, we can see that $b \leq 0$. Also, if we assume $x \in \text{int}(\mathcal{X})$, then $y = x + \varepsilon a \in \mathcal{X}$ for small $\varepsilon > 0$. Plugging this into (6), we see that $b = 0$ implies $a = 0$, which is a contradiction; therefore, $b < 0$. We can now rewrite (6) with $t = f(y)$ as

$$f(x) - f(y) \leq \frac{1}{|b|} a^T (x - y),$$

i.e. $a/|b|$ is a subgradient of f .

Finally, if f is convex and differentiable, it is not hard to show that $\nabla f(x) \in \partial f(x)$ by definition. □

2.1.2 first order optimality condition

We also have a nice first order optimality condition when dealing with convex functions.

Proposition 9 (First order optimality condition). *Let f be convex, and \mathcal{X} be a closed set on which f is differentiable. Then,*

$$x^* \in \arg \min_{x \in \mathcal{X}} f(x)$$

if and only if for all $y \in \mathcal{X}$,

$$\nabla f(x^*)^T (x^* - y) \leq 0.$$

Proof. If we first assume that $\nabla f(x^*)^T (x^* - y) \leq 0$ for all $y \in \mathcal{X}$, then since the gradient is a subgradient,

$$f(x^*) - f(y) \leq \nabla f(x^*)^T (x^* - y) \leq 0,$$

i.e. $f(x^*) \leq f(y)$ for all $y \in \mathcal{X}$.

Now, if we assume $x^* \in \arg \min_{x \in \mathcal{X}} f(x)$, we know that f is locally non-decreasing around x^* . Define $h(t) = f(x^* + t(y - x^*))$ for all $y \in \mathcal{X}$ – the rate of change of f along the line from x to y . We require $h'(0) \geq 0$ since x^* is a minimizer. Thus,

$$h'(0) = \nabla f(x^*)^T (y - x^*) \geq 0,$$

i.e. $\nabla f(x^*)^T (x^* - y) \leq 0$ for all $y \in \mathcal{X}$. □

We will see that the above proposition proves to be very useful when proving the convergence rates of projected gradient descent methods. Of course the above proposition holds with equality when x^* is an interior point, as $\nabla f(x^*) = 0$ in this case. However, it may also be the case that x^* is on the boundary of \mathcal{X} and not necessarily a minimum in the space in which \mathcal{X} is embedded, and this is the less-intuitive case that Proposition 9 handles well.

2.2 Black-box model

In the black-box model of computation, we assume that we know the constraint set \mathcal{X} but not the objective function $f : \mathcal{X} \rightarrow \mathbb{R}$. Nonetheless, we assume that we can make queries to an *oracle* and receive some information about f as output. Of particular interest to us is a **first order oracle**, which takes a point $x \in \mathcal{X}$ as input and outputs a subgradient of f at x . Of course, if f is convex, we will always be able to find a subgradient. We are interested in understanding the *oracle complexity* of convex optimization – the number of necessary and sufficient queries to the oracle to find an ε -approximate minima.

2.3 Projected gradient descent methods

We will now move into developing projected gradient descent algorithms for constrained optimization problems of the form

$$\min_{x \in \mathcal{X}} f(x),$$

where $f : \mathcal{X} \rightarrow \mathbb{R}$, and $\mathcal{X} \subset \mathbb{R}^n$ is the constraint set. If f is differentiable and $\mathcal{X} = \mathbb{R}^n$, we can write out the basic gradient descent method as

$$x_{t+1} = x_t - \eta \nabla f(x_t),$$

for some initial point $x_1 \in \mathbb{R}^n$ and step size $\eta > 0$. Methods of this type can obtain an *oracle complexity* that is independent of the dimension and are thus attractive in the high-dimensional setting.

However, we are interested in cases where the constraint set is a strict subset of \mathbb{R}^n and f may not be differentiable. We thus turn to a *projected subgradient descent* method instead, where each iteration performs the following: take a step in the direction of a subgradient of f , and then project this new point back onto the constraint set \mathcal{X} . We therefore begin by defining the projection operator and describe one of its properties.

Note that throughout this section, we will assume that the constraint set \mathcal{X} is compact and convex, and is contained in a Euclidean ball of radius B centred at $x_1 \in \mathcal{X}$. Furthermore, $\|\cdot\|$ denotes the Euclidean norm.

Definition 4 (Projection operator). *For all $y \in \mathbb{R}^n$, the projection operator on \mathcal{X} , $\Pi_{\mathcal{X}}$, is defined by*

$$\Pi_{\mathcal{X}}(y) = \arg \min_{x \in \mathcal{X}} \|x - y\|.$$

Lemma 1. *Let $x \in \mathcal{X}$ and $y \in \mathbb{R}^n$. Then,*

$$(\Pi_{\mathcal{X}}(y) - x)^T (\Pi_{\mathcal{X}}(y) - y) \leq 0,$$

which also implies $\|\Pi_{\mathcal{X}}(y) - x\|^2 + \|y - \Pi_{\mathcal{X}}(y)\|^2 \leq \|y - x\|^2$.

Proof. This is a direct consequence of Proposition 9 since $\Pi_{\mathcal{X}}(y)$ is a minimizer of $h_y(z) = \|y - z\|$, and $\nabla h_y(z) = (z - y)/\|z - y\|$. \square

2.3.1 L -Lipschitz functions

We now introduce projected subgradient descent for the case where the subgradients of $f(x)$ satisfy $\|g\| \leq L$, for all $x \in \mathcal{X}$. Note that this immediately implies f is L -Lipschitz continuous. The algorithm consists of two update steps at every iteration $t \geq 1$:

$$\begin{aligned} y_{t+1} &= x_t - \eta_t g_t, \text{ where } g_t \in \partial f(x_t), \\ x_{t+1} &= \Pi_{\mathcal{X}}(y_{t+1}). \end{aligned}$$

We state and prove the convergence of this method in the L -Lipschitz case below.

Theorem 2 (L -Lipschitz Projected Subgradient Descent). *Suppose \mathcal{X} is contained in a Euclidean ball of radius B centred at x_1 . Suppose also that for every $x \in \mathcal{X}$, the subgradients $g \in \partial f(x)$ satisfy $\|g\| \leq L$ and that f is convex. Then, the projected subgradient descent method with $\eta_s \equiv \eta = \frac{B}{L\sqrt{t}}$ satisfies*

$$f\left(\frac{1}{t} \sum_{s=1}^t x_s\right) - f(x^*) \leq \frac{LB}{\sqrt{t}} \quad \text{and} \quad f(x^o) - f(x^*) \leq \frac{LB}{\sqrt{t}}, \quad (7)$$

where $x^o \in \arg \min_{x \in \{x_1, \dots, x_t\}} f(x)$. Moreover, with $\eta_s = \frac{B}{L\sqrt{s}}$, then $\exists c > 0$ (for instance, $c = 2(1 + \log 2)$) such that

$$f\left(\left(\sum_{s=\lceil t/2 \rceil+1}^t \eta_s\right)^{-1} \sum_{s=\lceil t/2 \rceil+1}^t \eta_s x_s\right) - f(x^*) \leq c \frac{LB}{\sqrt{t}} \quad \text{and} \quad f(x^o) - f(x^*) \leq c \frac{LB}{\sqrt{t}}. \quad (8)$$

Proof. Recall that $2a^T b = \|a\|^2 + \|b\|^2 - \|a - b\|^2$. Then, for any $1 \leq s \leq t$,

$$\begin{aligned} f(x_s) - f(x^*) &\leq g_s^T (x_s - x^*) \\ &= \frac{1}{\eta} (x_s - y_{s+1})^T (x_s - x^*) \\ &= \frac{1}{2\eta} (\|x_s - x^*\|^2 + \|x_s - y_{s+1}\|^2 - \|y_{s+1} - x^*\|^2) \\ &= \frac{1}{2\eta} (\|x_s - x^*\|^2 - \|y_{s+1} - x^*\|^2) + \frac{\eta}{2} \|g_s\|^2. \end{aligned}$$

Now, from Lemma 1, we know that $\|y_{s+1} - x^*\| \geq \|x_{s+1} - x^*\|$. Therefore, summing from $s = 1$ to t , we get

$$\frac{1}{t} \sum_{s=1}^t (f(x_s) - f(x^*)) \leq \frac{1}{2\eta t} (\|x_1 - x^*\|^2 - \|x_{t+1} - x^*\|^2) + \frac{\eta}{2} L^2 \leq \frac{B^2}{2\eta t} + \frac{\eta L^2}{2}.$$

Selecting $\eta = \frac{B}{L\sqrt{t}}$ to minimize the right-hand side of the above inequality gives the first result in (7) (since $f\left(\frac{1}{t} \sum_{s=1}^t x_s\right) \leq \frac{1}{t} \sum_{s=1}^t f(x_s)$ by Jensen's inequality). Clearly, $f(x^o) \leq \frac{1}{t} \sum_{s=1}^t f(x_s)$, proving the second result of (7).

Now consider the case of an adaptive step size η_s . The above derivation yields

$$f(x_s) - f(x^*) \leq \frac{1}{2\eta_s} (\|x_s - x^*\|^2 - \|y_{s+1} - x^*\|^2) + \frac{\eta_s}{2} \|g_s\|^2.$$

If we want to apply the same argument as above and get a telescoping sum with cancellations, we need to take a weighted sum weighted by η_s . Namely, replacing $t^{-1} \sum_{s=1}^t$ with $(\sum_{s=1}^t \eta_s)^{-1} \sum_{s=1}^t \eta_s$ we get

$$\left(\sum_{s=1}^t \eta_s \right)^{-1} \sum_{s=1}^t \eta_s (f(x_s) - f(x^*)) \leq \left(\sum_{s=1}^t \eta_s \right)^{-1} \left(\frac{B^2}{2} + \left(\sum_{s=1}^t \eta_s^2 \right) \frac{L^2}{2} \right),$$

which reduces to the previous result when $\eta_s \equiv \eta$. We want the right-hand-side to go to zero as t increases, so we need both $\sum \eta_s \rightarrow \infty$ and $\frac{\sum \eta_s^2}{\sum \eta_s} \rightarrow 0$. This is the case if we take $\eta_s = \frac{K}{\sqrt{s}}$, as $\sum_{s=1}^t \eta_s \geq c_1 K \sqrt{t}$ (e.g., $c_1 = 1$) and $\sum_{s=1}^t \eta_s^2 \leq c_2 K^2 \log t$ (e.g., $c_2 = 1 + 1/\log 2$ if $t \geq 2$, using that $\sum_{s=1}^t 1/s \leq 1 + \int_{s=0}^t \frac{1}{s} ds = 1 + \log t \leq c_2 \log t$). We can then choose $K = \frac{B}{L}$ such that

$$\left(\sum_{s=1}^t \eta_s \right)^{-1} \sum_{s=1}^t \eta_s (f(x_s) - f(x^*)) \leq \frac{B^2}{2c_1 K \sqrt{t}} + \frac{c_2 K L^2 \log t}{2c_1 \sqrt{t}} \leq \left(\frac{1+c_2}{2c_1} \right) LB \sqrt{\frac{\log t}{t}}.$$

To get rid of the log term, we note that if we only sum from $\lceil t/2 \rceil + 1$ to t , for $t \geq 3$, we have $\sum_{s=\lceil t/2 \rceil + 1}^t \eta_s \geq c'_1 K \sqrt{t}$ (e.g., $c'_1 = 1/4$, as $\sum_{s=\lceil t/2 \rceil + 1}^t 1/\sqrt{s} \geq \frac{t-1}{2\sqrt{t}} = \frac{\sqrt{t}}{2}(1 - 1/t) \geq \frac{\sqrt{t}}{4}$) and $\sum_{s=\lceil t/2 \rceil + 1}^t \eta_s^2 \leq c'_2 K^2$ (e.g., $c'_2 = \log 2$ using that $\sum_{s=\lceil t/2 \rceil + 1}^t \frac{1}{s} \leq \int_{t/2}^t \frac{1}{s} ds = \log 2$). Therefore, we finally have that

$$\min_{1 \leq s \leq t} f(x_s) - f(x^*) \leq \min_{\lceil t/2 \rceil + 1 \leq s \leq t} f(x_s) - f(x^*) \leq \left(\sum_{s=\lceil t/2 \rceil + 1}^t \eta_s \right)^{-1} \sum_{s=\lceil t/2 \rceil + 1}^t \eta_s (f(x_s) - f(x^*)) \leq c \frac{LB}{\sqrt{t}},$$

with $c = \left(\frac{1+c'_2}{2c'_1} \right)$, where we used that the minimum element of a set is always less or equal to a convex combination of the elements. The proof of both results in (8) follows again by Jensen's inequality. \square

The result of (8) is promising since we would rather use an adaptive step size than one that depends on the total number of iterations t , to be set and fixed in advance, i.e., prior to running the algorithm. Unfortunately, both step sizes still depend on B and L – quantities which may not be known. The results in Theorem 2 demonstrate that the projected subgradient method for convex and L -Lipschitz functions exhibits a convergence rate of $O\left(\frac{BL}{\sqrt{t}}\right)$. We can also phrase this in terms of *oracle complexity*: as at each iteration we make a constant (in fact, one) number of calls to the oracle, then to achieve ε -convergence, we require $\frac{BL}{\sqrt{t}} \leq \varepsilon$, or $t \geq \frac{B^2 L^2}{\varepsilon^2}$.

2.3.2 β -smooth functions

Now, we move to the case of a β -smooth convex function. Recall a function $f : \mathcal{X} \rightarrow \mathbb{R}$ is β -smooth if, for all $x, y \in \mathcal{X}$, we have $\|\nabla f(x) - \nabla f(y)\| \leq \beta \|x - y\|$. We show some auxiliary results first for convex and β -smooth functions – deferring to [3] for the proofs – before deriving the convergence rate of projected subgradient descent with $\eta = \frac{1}{\beta}$.

Lemma 2. *Let $f : \mathcal{X} \rightarrow \mathbb{R}$ be a convex and β -smooth function. Then, for all $x, y \in \mathcal{X}$, we have*

$$f(x) - f(y) - \nabla f(y)^T(x - y) \leq \frac{\beta}{2} \|x - y\|^2.$$

Proof. Refer to the proof in [3, Lemma 3.4]. \square

Lemma 3. Let $x, y \in \mathcal{X}$, $x^+ = \Pi_{\mathcal{X}}\left(x - \frac{1}{\beta}\nabla f(x)\right)$, and $g_{\mathcal{X}}(x) = \beta(x - x^+)$. Then, we have the following:

$$f(x^+) - f(y) \leq g_{\mathcal{X}}(x)^T(x - y) - \frac{1}{2\beta}\|g_{\mathcal{X}}(x)\|^2.$$

Proof. Refer to the proof in [3, Lemma 3.6]. □

Theorem 3 (β -Smooth Projected Subgradient Descent). Let $f : \mathcal{X} \rightarrow \mathbb{R}$ be convex and β -smooth on \mathcal{X} . Also, suppose \mathcal{X} is contained in a Euclidean ball of radius B centred at x_1 . Then, the projected subgradient descent method with $\eta = \frac{1}{\beta}$ satisfies

$$f(x_t) - f(x^*) \leq \frac{3\beta B^2 + f(x_1) - f(x^*)}{t}. \quad (9)$$

Proof. From Lemma 3 and since $x_{s+1} = \Pi_{\mathcal{X}}(x_s - \frac{1}{\beta}\nabla f(x_s))$, we have the following:

$$\begin{aligned} f(x_{s+1}) - f(x_s) &\leq g_{\mathcal{X}}(x_s)^T(x_s - x_s) - \frac{1}{2\beta}\|g_{\mathcal{X}}(x_s)\|^2 = -\frac{1}{2\beta}\|g_{\mathcal{X}}(x_s)\|^2, \text{ and} \\ f(x_{s+1}) - f(x^*) &\leq g_{\mathcal{X}}(x_s)^T(x - x^*) \leq \|g_{\mathcal{X}}(x_s)\| \cdot \|x_s - x^*\|, \end{aligned}$$

since $f(x_{s+1}) \geq f(x^*)$. Also, we can show that $\|x_s - x^*\|$ is decreasing with s : from Lemma 3, we have $g_{\mathcal{X}}(x_s)^T(x_s - x^*) \geq \frac{1}{2\beta}\|g_{\mathcal{X}}(x_s)\|^2$, and thus

$$\begin{aligned} \|x_{s+1} - x^*\|^2 &= \|x_s - \frac{1}{\beta}g_{\mathcal{X}}(x_s) - x^*\|^2 \\ &= \|x_s - x^*\|^2 - \frac{2}{\beta}g_{\mathcal{X}}(x_s)^T(x_s - x^*) + \frac{1}{\beta^2}\|g_{\mathcal{X}}(x_s)\|^2 \leq \|x_s - x^*\|^2. \end{aligned}$$

We can therefore bound the difference $f(x_{s+1}) - f(x^*)$ in terms of the difference at the previous iterate:

$$\begin{aligned} f(x_{s+1}) - f(x^*) &= (f(x_{s+1}) - f(x_s)) + (f(x_s) - f(x^*)) \\ &\leq f(x_s) - f(x^*) - \frac{1}{2\beta}\|g_{\mathcal{X}}(x_s)\|^2 \\ &\leq f(x_s) - f(x^*) - \frac{\|g_{\mathcal{X}}(x_s)\|^2\|x_s - x^*\|^2}{2\beta\|x_1 - x^*\|^2} \\ &\leq f(x_s) - f(x^*) - \frac{(f(x_{s+1}) - f(x^*))^2}{2\beta\|x_1 - x^*\|^2}. \end{aligned}$$

Thus, we can prove (9) using induction. It is trivial to show the base case $t = 1$. Then, assuming it is true for $t = s$,

$$\begin{aligned} f(x_{s+1}) - f(x^*) &\leq f(x_s) - f(x^*) - \frac{(f(x_{s+1}) - f(x^*))^2}{2\beta\|x_1 - x^*\|^2} \\ &\leq \frac{3\beta B^2 + f(x_1) - f(x^*)}{s}, \text{ by the inductive hypothesis} \\ &\leq \frac{3\beta B^2 + f(x_1) - f(x^*)}{s+1}. \end{aligned}$$

Therefore, (9) is true for all $t \in \mathbb{N}$. □

The above theorem demonstrates that for β -smooth convex functions, the error in estimating the optimal function value $O\left(\frac{\beta B^2}{t}\right)$, corresponding to an oracle complexity of $O\left(\frac{\beta B^2}{\varepsilon}\right)$. We notice that the error rate decreasing faster in t in this case than in the Lipschitz case, but the dependence on B^2 instead of B is more loose, and we will see in subsection 2.4 that we cannot compare β and L directly. We also note here that the step size η depends on β , which can be difficult to find in practice. As in the Lipschitz case, we again have no explicit reference to the underlying dimension n , although both B and β implicitly depend on n .

2.4 Remark on convexity, strong convexity, smoothness, and Lipschitz continuity

Finally, having shown convergence results for convex β -smooth and L -Lipschitz functions, it is important to note the geometric connection between these types of functions and convex functions. Recall the Taylor series expansion of $f(y)$ around x :

$$f(y) \approx f(x) + \nabla f(x)^T(y - x) + \frac{1}{2}(y - x)^T \nabla^2 f(x)(y - x) + \dots$$

Convex functions are uniformly bounded *below* by an hyperplane that can be constructed at any point x :

$$f(y) \geq f(x) + \nabla f(x)^T(y - x),$$

and α -strongly convex functions are uniformly bounded *below* by this hyperplane and a quadratic:

$$f(y) \geq f(x) + \nabla f(x)^T(y - x) + \frac{\alpha}{2}\|y - x\|^2.$$

On the other hand, β -smooth functions are uniformly bounded *above* by this hyperplane and a quadratic:

$$f(y) \leq f(x) + \nabla f(x)^T(y - x) + \frac{\beta}{2}\|y - x\|^2.$$

Finally, L -Lipschitz functions are uniformly bounded *above and below* by a double cone:

$$f(x) - L\|y - x\| \leq f(y) \leq f(x) + L\|y - x\|.$$

Another important point to note is the relative independence of β -smoothness and Lipschitz continuity. Consider the case where $f(x) = x^2$ – clearly, this is β -smooth for $\beta = 2$ (and α -strongly convex with $\alpha = 2$). However, it is not Lipschitz continuous, as we cannot hope to uniformly upper-bound a quadratic function by a line. On the other hand, consider the hinge function $f(x) = \max(0, 1 + x)$. It is easy to see that this is Lipschitz continuous with $L = 1$, but not β -smooth for any β . Thus, neither condition implies the other.

3 Lower bounds for oracle complexity

Speaker: Dominic Richards, 26/10/2017.

3.1 Week 2 Recap

Recall the objective is to minimise some convex function $f : \mathcal{X} \rightarrow \mathbb{R}$, being phrased as the following optimisation problem

$$\min f(x) \tag{10}$$

$$\text{s.t. } x \in \mathcal{X} \tag{11}$$

where \mathcal{X} has the assumption $\sup_{x \in \mathcal{X}} \|x\|_2 \leq R$, that is we can enclose the optimisation space inside a Euclidean ball of size R . The optimal will be denoted $x^* = \arg \min_{x \in \mathcal{X}} f(x)$.

An assortment of assumptions can be placed upon f , the following 3 are of most interest

1. L-Lipschitz: $|f(x) - f(y)| \leq L\|x - y\|_2$ for any $x, y \in \mathbb{R}^n$ ($\|\nabla f(x)\|_2 \leq L$).
2. β -smooth: $\|\nabla f(x) - \nabla f(y)\|_2 \leq \beta\|x - y\|_2$ for any $x, y \in \mathbb{R}^n$ ($\nabla^2 f(x) \preceq \beta I$ for any $x, y \in \mathbb{R}^n$)
3. α -Strong convexity: $f(x) - f(y) \leq \nabla f(x)^T(x - y) - \frac{\alpha}{2}\|x - y\|_2^2$ for any $x, y \in \mathbb{R}^n$ ($\nabla^2 f(x) \succeq \alpha I$ for any $x \in \mathbb{R}^n$).

Recall that α -Strong convexity may not be reasonable in applied problems where the sample size is small, due to is aligning implying the empirical covariance matrix is invertible. For more information on this look to proposition 2 from the notes accompanying this reading group.

Now we recall some results from the previous chapter regarding projected gradient descent. The routine, denoting the set of sub gradients for $f(x)$ as $\partial f(x)$, is the following

$$y_{t+1} = x_t - \eta g_t \quad \text{where } g_t \in \partial f(x_t) \tag{12}$$

$$x_{t+1} = \Pi_{\mathcal{X}}(y_{t+1}) \tag{13}$$

where the function $\Pi_{\mathcal{X}}(y_{t+1})$ projects the point y_{t+1} back into the constraint set \mathcal{X} . The rate at the above routine finds x^* depends upon which of the assumptions above f satisfies. We now list down the bounds between the the sequence of points produced from the above routine and the optimal x^* under different conditions on f .

L-Lipschitz and Convex from Theorem 3.2 from [3] with $\eta = \frac{R}{L\sqrt{t}}$

$$f\left(\frac{1}{t} \sum_{s=1}^t x_s\right) - f(x^*) \leq \frac{RL}{\sqrt{t}} \tag{14}$$

giving a complexity of $O(RL/\sqrt{t})$

β -Smooth and Convex from Theorem 3.7 in [3] with $\eta = \frac{1}{\beta}$

$$f(x_t) - f(x^*) \leq \frac{3\beta\|x_1 - x^*\|^2 + f(x_1) - f(x^*)}{t} \tag{15}$$

giving a complexity of $O\left(\frac{R^2\beta}{t}\right)$.

L-Lipschitz and α -strongly Convex from Theorem 3.9 in [3] with $\eta_s = \frac{2}{\alpha(s+1)}$, that is the gradient step now depends upon time, we get

$$f\left(\sum_{s=1}^t \frac{2s}{t(t+1)} x_s\right) - f(x^*) \leq \frac{2L^2}{\alpha(t+1)} \quad (16)$$

giving a complexity of $O\left(\frac{L^2}{\alpha(t+1)}\right)$.

β -Smooth and α -strongly Convex from Theorem 3.10 in [3] with $\eta = \frac{1}{\beta}$ we have

$$\|x_{t+1} - x^*\|^2 \leq \exp\left(-\frac{\alpha t}{\beta}\right) \|x_1 - x^*\|^2 \quad (17)$$

giving a complexity of $O\left(R^2 \exp\left(-\frac{\alpha t}{\beta}\right)\right)$.

3.2 Week 3 - Lower Bounds

To prove lower complexity bounds a "sufficiently hard" f , satisfying the various conditions, must be found, that, when giving a black-box procedure a fixed number of first order oracle calls, will remain a fixed distance away from its optimum. An example of a black-box procedure being the projected gradient descent of previously - taking a position and sub gradient (x_t, g_t) $g_t \in \partial f(x_t)$ and returning the next position $x_{t+1} = \Pi_{\mathcal{X}}(x_t - \eta g_t)$. Recalling that a first order oracle call at $f(x)$ returns to us a sub-gradient $g \in \partial f(x)$.

Generalising this, given a history $(x_1, g_1, \dots, x_t, g_t)$ such that $g_s \in \partial f(x_s)$, a black-box procedure will be a mapping $(x_1, g_1, \dots, x_t, g_t) \rightarrow x_{t+1}$. Letting $x_1 = 0$, we will assume that the black-box procedure, for any $t \geq 0$, returns a position in the span of the gradients

$$x_{t+1} \in \text{Span}(g_1, \dots, g_t). \quad (18)$$

Additionally we denote the standard basis of \mathbb{R}^n as e_1, \dots, e_n , and the Euclidean ball of radius R as $B_2(R) = \{x \in \mathbb{R}^n : \|x\| < R\}$.

Now for any $t \leq n$ we will show there exists an f that will remain bounded away from its optimal within the first t calls to a black-box procedure satisfying (18). Noting that if the number of oracle calls grows beyond the dimension ($t > n$) Vaidya method from Chapter 2 becomes viable, achieving ϵ accuracy in $n \log(\frac{Rn}{r\epsilon})$ first order oracle calls.

The remainder of this section is as follows: first lower oracle complexity bounds for various f are listed, after which the proof for the β -Smooth and Convex case is provided. The proof for the L -Lipschitz α -Strong Convex case being omitted due to it being similar in spirit to the β -Smooth case. After which we will find out there a gap between the rates achieved by projected gradient descent and the proven complexity lower bounds, suggesting new methods can be found in order to improve rates. Before moving on we highlight an additional source [2, 75-76] which included some interesting relevant points.

Theorem 4. *Lower Bound for L-Lipschitz and Convex / α -Convex*

Let $t \leq n$, $L, R > 0$. There exists an L-Lipschitz and Convex f such that for any black-box procedure satisfying (18)

$$\min_{1 \leq s \leq t} f(x_s) - \min_{x \in B_2(R)} f(x) \geq \frac{RL}{2(1 + \sqrt{t})} \quad (19)$$

thus giving oracle complexity of $\Omega\left(\frac{1}{\epsilon^2}\right)$. Moreover if f is α -strongly Convex

$$\min_{1 \leq s \leq t} f(x_s) - \min_{x \in B_2(R)} f(x) \geq \frac{L^2}{8\alpha t} \quad (20)$$

giving oracle complexity of $\Omega\left(\frac{1}{\epsilon}\right)$.

Remark: These rates are optimal in the case of projected gradient descent.

Proof: See Theorem 3.13 [3].

Theorem 5. *Lower Bound for β -Smooth and Convex*

Let $t \leq (n-1)/2, \beta > 0$. There exists a β -smooth convex f such that for any black-box procedure satisfying (18)

$$\min_{1 \leq s \leq t} f(x_s) - \min_{x \in B_2(R)} f(x) \geq \frac{3\beta}{32} \frac{\|x_1 - x^*\|^2}{(t+1)^2} \quad (21)$$

giving a lower oracle complexity bound of $\Omega\left(\frac{1}{\sqrt{\epsilon}}\right)$.

Proof Adapted from [3] Theorem 3.14:

Let $A_k \in \mathbb{R}^{n \times n}$ be a matrix defined by

$$(A_k)_{i,j} = \begin{cases} 2, & i = j, i \leq k \\ -1, & j \in \{i-1, i+1\}, i \leq k, j \neq k+1 \\ 0, & \text{Otherwise} \end{cases}$$

which can alternatively be represented in the standard basis as

$$A_k = 2 \sum_{i=1}^k e_i e_i^T - \sum_{i=1}^{k-1} e_i e_{i+1}^T - \sum_{i=2}^{k-1} e_{i+1} e_i^T \quad (22)$$

noting that $0 \preceq A_k \preceq 4I_n$ since

$$x^T A_k x = 2 \sum_{i=1}^k x(i)^2 - 2 \sum_{i=1}^{k-1} x(i)x(i+1) = x(1)^2 + x(k)^2 + \sum_{i=1}^{k-1} (x(i) - x(i+1))^2.$$

Consider now the β -smooth convex function

$$f(x) = \frac{\beta}{8} x^T A_{2t+1} x - \frac{\beta}{4} x^T e_1$$

which has the sub gradient $\partial f(x) = \frac{\beta}{4} A_{2t+1} x - \frac{\beta}{4} e_1$. As $x_1 = 0$ we have $\partial f(x_1) = -\frac{\beta}{4} e_1$, and due to (18), $x_2 = \eta_{21} e_1$ for $\eta_{21} \in \mathbb{R}$. Next iteration we have $\partial f(x_2) = \frac{\beta}{4} (A_{2t+1} x_2 - e_1)$ which, using the representation (22), is now in the direction of e_2 . To see this consider the following

$$\begin{aligned} A_{2t+1} x_2 &= \eta_{21} A_k e_1 = \eta_{21} \left(2 \sum_{i=1}^{2t+1} e_i e_i^T - \sum_{i=1}^{2t} e_i e_{i+1}^T - \sum_{i=2}^{2t} e_{i+1} e_i^T \right) e_1 \\ &= \eta_{21} (2e_1 - e_2) \end{aligned}$$

as $e_i^T e_1 = 0$ if $i \neq 1$. Therefore we can deduce that $\text{Span}(e_1, \partial f(x_2)) = \text{Span}(e_1, e_2)$.

Proceeding inductively for iterations $2 \leq s \leq t$, we have $x_s \in \text{Span}(e_1, \dots, e_{s-1})$, and therefore $x_s = \sum_{i=1}^{s-1} \eta_{s-1,i} e_i$. Once again $\partial f(x_s)$ will contain

$$\begin{aligned}
A_{2t+1}x_s &= \left(2 \sum_{i=1}^{2t+1} e_i e_i^T - \sum_{i=1}^{2t} e_i e_{i+1}^T - \sum_{i=2}^{2t} e_{i+1} e_i^T \right) \left(\sum_{j=1}^{s-1} \eta_{s-1,j} e_j \right) \\
&= \sum_{j=1}^{s-1} \eta_{s-1,j} \left(2 \sum_{i=1}^{2t+1} e_i e_i^T - \sum_{i=1}^{2t} e_i e_{i+1}^T - \sum_{i=2}^{2t} e_{i+1} e_i^T \right) e_j \\
&= \sum_{j=1}^{s-1} \eta_{s-1,j} (2e_j - e_{j-1} - e_{j+1})
\end{aligned}$$

which most importantly is now in the direction of e_s due to element e_{j+1} under the sum, meaning that $\text{Span}(e_1, \dots, e_{s-1}, \partial f(x_s)) = \text{Span}(e_1, \dots, e_s)$.

Intuitively, due to the right most sum in (22), one extra co-ordinate is explored per iteration. This means, for some $s \leq t$, x_s will be zero in the co-ordinates not yet to explore, that is $x_s(i) = 0$ for $i = s, \dots, n$. Therefore $x_s^T A_{2t+1} x_s = x_s^T A_s x_s$, which means the best we can do in the first s iterations is find the optimal of a restricted version of f , namely $f_s(x)$, defined for some k as

$$f_k(x) = \frac{\beta}{8} x A_k x - \frac{\beta}{4} x^T e_1. \quad (23)$$

The objective is to bound the difference between the optimal values of the restricted f_s and global f , thus proving the black box method can only do so well in t iterations. Denoting $f^* = \inf_{x \in \mathcal{X}} f(x)$, consider the following set of inequalities

$$f(x_s) - f^* = f_s(x_s) - f_{2t+1}^* \geq f_s^* - f_{2t+1}^* \geq f_t^* - f_{2t+1}^* \quad (24)$$

To see $f_s^* \geq f_t^*$ observe that

$$\begin{aligned}
f_t(x) &= \sum_{i=1}^s x(i) - 2 \sum_{i=1}^{s-1} x(i)x(i+1) + 2 \sum_{i=s+1}^t x(i)^2 - 2 \sum_{i=s}^{t-1} x(i)x(i+1) \\
&= f_s(x) + x(s+1)^2 + x(t)^2 + \sum_{i=s+1}^{t-1} (x(i) - x(i+1))^2 - 2x(s)x(s+1)
\end{aligned}$$

which when plugging in the optimal point for f_s can attain $f_t(x_s^*) = f_s(x_s^*) = f_s^*$ as $x_s^*(i) = 0$ for $i = s+1, \dots, n$.

We must now explicitly find the minimiser x_k^* for f_k , its norm, and the corresponding objective f_k^* . To find x_k^* we have $\partial f_k(x) = 0 \implies A_k x = e_1$, and since $x_k^* \in \text{Span}(e_1, \dots, e_k)$, the solution becomes $x_k^*(i) = 1 - \frac{i}{k+1}$ for $i = 1, \dots, k$. We then immediately get

$$f_k^* = -\frac{\beta}{8} \left(1 - \frac{1}{k+1} \right). \quad (25)$$

With the norm of x_s^* then becoming

$$\|x_k^*\| = \sum_{i=1}^k \left(1 - \frac{i}{k+1} \right)^2 = \sum_{i=1}^k \left(\frac{i}{k+1} \right)^2 \leq \frac{k+1}{3}. \quad (26)$$

Finally bringing together (24), (25), (26) we get

$$f(x_s) - f^* \geq f_t^* - f_{2t+1}^* = \frac{\beta}{8} \left(\frac{1}{t+1} - \frac{1}{2t+2} \right) \geq \frac{3\beta}{32} \frac{\|x_{2t+1}^*\|^2}{(t+1)^2}$$

noting that as the right hand side does not depending upon x_s , a minimum can be taken. \square

To make comparison between the lower bound rates as well as those obtained by projected gradient descent, we look to oracle complexities contained in Figure 1.

		Upper Bound (PGD)	Lower Bound
Convex	L -Lipschitz	$O\left(\frac{1}{\epsilon^2}\right)$	$\Omega\left(\frac{1}{\epsilon^2}\right)$
	β -Smooth	$O\left(\frac{1}{\epsilon}\right)$	$\Omega\left(\frac{1}{\sqrt{\epsilon}}\right)$
α -Strong Convex	L -Lipschitz	$O\left(\frac{1}{\epsilon}\right)$	$\Omega\left(\frac{1}{\epsilon}\right)$
	β -Smooth	$O\left(\frac{\beta}{\alpha} \log(\epsilon^{-1})\right)$	$\Omega\left(\sqrt{\frac{\beta}{\alpha}} \log(\epsilon^{-1})\right)$

Figure 1: Oracle complexity- order of iterations t required for $f(x_t) - f^* \leq \epsilon$. Source for lower bound in the β -Smooth α -Strong Convex case from Theorem 3.15 [3]. Upper Bound is oracle complexity of (PGD) Projected Gradient Descent.

Observe that there is a gap in the upper and lower bounds in the case of β -smooth functions, specifically an order $\frac{1}{\sqrt{\epsilon}}$ and $\sqrt{\frac{\beta}{\alpha}}$ for Convex and α -Strong Convex functions respectively. This suggests there are more optimal black box procedure over projected gradient descent that could close the complexity gap.

4 Application: Boosting

5 Non-Euclidean setting: mirror descent

6 Acceleration by coupling gradient descent and mirror descent

7 Non-Euclidean setting: Frank-Wolfe

8 Stochastic oracle model

Assume that we want to solve the following problem:

$$\begin{aligned} & \text{minimize} && f(x) \\ & \text{subject to} && x \in \mathcal{X}, \end{aligned} \tag{27}$$

where f is a convex function, possibly not known. The first order *stochastic* oracle model defines the framework where given $x \in \mathcal{X}$ an oracle yields back a random variable G that is an unbiased estimator of a subgradient of f at x , namely, $\mathbf{E}[G] \in \partial f(x)$. If X is a random variable, the oracle yields back a random variable G that is an unbiased estimator of a subgradient of f at X conditionally on X , namely, $\mathbf{E}[G|X] \in \partial f(X)$.

L -Lipschitz functions

We analyze the behavior of the projected gradient descent algorithm to solve problem (27) when we replace exact knowledge of subgradients of f with unbiased estimates of them. For a given initial point $X_1 \in \mathcal{X}$, possibly random, and a given collection of step sizes η_1, η_2, \dots , the stochastic projected gradient descent is defined by the sequence of random variables generated according to the following update:

$$\begin{aligned} Y_{s+1} &= X_s - \eta_s G_s, \\ X_{s+1} &= \Pi_{\mathcal{X}}(Y_{s+1}). \end{aligned}$$

Here, conditionally on X_s , the random variable G_s is an unbiased estimator of the subgradient of the function f at X_s , namely,

$$\mathbf{E}[G_s|X_s] \in \partial f(X_s).$$

We state and prove the convergence of this method in the L -Lipschitz case.

Theorem 6 (*L -Lipschitz Stochastic Projected Subgradient Descent*). *Let f be convex. Suppose \mathcal{X} is contained in a Euclidean ball of radius B centred at X_1 . Suppose that for every $X \in \mathcal{X}$ the stochastic oracle yields an unbiased estimator of the subgradient of f at X bounded in L_2 , namely, $\mathbf{E}[G|X] \in \partial f(X)$ and $\mathbf{E}[\|G\|^2] \leq L^2$. Then, the projected subgradient descent method with $\eta_s \equiv \eta = \frac{B}{L\sqrt{t}}$ satisfies*

$$\mathbf{E}f\left(\frac{1}{t} \sum_{s=1}^t X_s\right) - f(x^*) \leq \frac{LB}{\sqrt{t}}. \tag{28}$$

Proof. For any $1 \leq s \leq t$ we have

$$f(X_s) - f(x^*) \leq \mathbf{E}[G_s|X_s]^T (X_s - x^*) = \mathbf{E}[G_s^T (X_s - x^*)|X_s].$$

Proceeding as in the proof of Theorem 2, we find

$$G_s^T (X_s - x^*) \leq \frac{1}{2\eta} (\|X_s - x^*\|^2 - \|X_{s+1} - x^*\|^2) + \frac{\eta}{2} \|G_s\|^2.$$

Taking the expectation, we get

$$\mathbf{E}f(X_s) - f(x^*) \leq \mathbf{E}[G_s^T (X_s - x^*)] \leq \frac{1}{2\eta} (\mathbf{E}\|X_s - x^*\|^2 - \mathbf{E}\|X_{s+1} - x^*\|^2) + \frac{\eta}{2} \mathbf{E}[\|G_s\|^2],$$

and using the assumption $\mathbf{E}[\|G_s\|^2] \leq L^2$ we get

$$\frac{1}{t} \sum_{s=1}^t (\mathbf{E}f(X_s) - f(x^*)) \leq \frac{1}{2\eta t} (\mathbf{E}\|X_1 - x^*\|^2 - \mathbf{E}\|X_{t+1} - x^*\|^2) + \frac{\eta}{2} L^2 \leq \frac{B^2}{2\eta t} + \frac{\eta L^2}{2}.$$

Selecting $\eta = \frac{B}{L\sqrt{t}}$ to minimize the right-hand side of the above inequality gives the first result in (7) (since $f\left(\frac{1}{t} \sum_{s=1}^t X_s\right) \leq \frac{1}{t} \sum_{s=1}^t f(X_s)$ by Jensen's inequality). \square

Theorem 6 shows that, in expectation, the stochastic projected subgradient descent method yields the same convergence guarantees as the deterministic counterpart analyzed in Theorem 2. In particular, the oracle complexity is the same³: to get an accuracy ε , both methods requires $O(1/\varepsilon^2)$ calls to their respective oracles. The main advantage of the stochastic version lies in the fact that in some applications the *computational* complexity involved in having access to a stochastic oracle is much cheaper than in the deterministic case. We now show that the stochastic model yields substantial computational saving in machine learning.

8.1 Multiple passes over the data

TO DO.

8.2 Single pass over the data

We now show how the first order stochastic oracle model allows us to deal directly with expected risk minimization without invoking the empirical risk minimization paradigm. Let us recall the original problem that motivates us in Section 1, namely, the expected risk minimization:

$$\begin{aligned} & \text{minimize} && r(x) = \mathbf{E}\ell(x^T \Phi(W), Y) \\ & \text{subject to} && x \in \mathcal{X}. \end{aligned}$$

The assumption here is that we know the loss function ℓ (indeed, we can choose it!) and the constraint set \mathcal{X} , but we do not know the distribution of (W, Y) . We only have access to m i.i.d. samples $(W_1, Y_1), \dots, (W_m, Y_m)$ from this unknown distribution. So we do not know the function r that we want to minimize, and in particular we can not operate in the deterministic first order oracle model discussed in the previous weeks as for a given $x \in \mathcal{X}$ we do not have access to a subgradient in $\partial r(x)$. On the other hand, given $x \in \mathcal{X}$ we can have access to an unbiased estimator of a subgradient of r evaluated at x . In fact, given the function $x \rightarrow R_i(x) := \ell(x^T \Phi(W_i), Y_i)$, which is known to us, we can compute a subgradient of R_i at x . This is a random variable $G_i \in \partial R_i(x)$ that satisfies $\mathbf{E}G_i \in \partial r(x)$. The same is true if we want to get an estimate of the subgradient of r at $X \in \mathcal{X}$ when X is a random variable *independent* of (W_i, Y_i) . In fact, in this case we can evaluate a subgradient of R_i at X , and this random variable $G_i \in \partial R_i(X)$ satisfies $\mathbf{E}[G_i|X] \in r(X)$.⁴ Hence, we satisfy the assumption of the first order stochastic oracle model. At the same time, as we have m independent data points at our disposal, we can have access to at most m independent unbiased estimators of subgradients evaluated at possibly different locations in \mathcal{X} . In other words, the requirement of independence restricts us to a *single pass* over the data, which is not as general as in the stochastic block model defined above where we can have how many queries to the oracle as we want.

It is easy to check that under the assumptions of Proposition 3, Theorem 6 yields the following convergence guarantees for the stochastic projected descent method:

$$\mathbf{E}r(\hat{X}_m) - r(x^*) \leq \frac{GL_{\text{loss}}B}{\sqrt{m}},$$

with $\hat{X}_m = \frac{1}{m} \sum_{i=1}^m X_i$. In other word, we can apply the stochastic gradient descent algorithm to *directly* minimize the expected risk r , without invoking the empirical risk minimization paradigm, i.e., without breaking the problem into statistics and optimization as outlined in Section 1. The computational savings are clear. If computing a

³Note that different notions of accuracy are used, however, as we consider the expected value of the stochastic method.

⁴Note that if X is random, then there are two sources of randomness in G_i : one source is X itself, the other is the data point (W_i, Y_i) . The statement $\mathbf{E}[G_i|X] \in r(X)$ holds if X and (W_i, Y_i) are independent.

subgradient for each functions R_i costs $O(1)$, then the computational complexity of stochastic gradient descent to achieve precision ε (in expectation) is of order $O(1/\varepsilon^2)$. On the other hand, if we apply the deterministic gradient descent method to minimize the empirical risk R up to precision $1/\sqrt{m}$, as discussed in Section 1 and in Remark 1, then we see that the computational complexity is $O(m/\varepsilon^2)$, as we need $O(1/\varepsilon^2)$ calls to the deterministic oracle but each call costs $O(m)$ base iterations, as $R(x) := \frac{1}{m} \sum_{i=1}^m R_i(x)$.

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