

Convexification of Learning from Constraints

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Abstract

Regularized empirical risk minimization with **constrained labels** (in contrast to fixed labels) is a remarkably general abstraction of learning. For common loss and regularization functions, this optimization problem assumes the form of a mixed integer program (MIP) whose objective function is non-convex. In this form, the problem is resistant to standard optimization techniques. We construct MIPs with the same solutions whose objective functions are **convex**. Specifically, we characterize the tightest convex extension of the objective function, given by the Legendre-Fenchel biconjugate. Computing values of this tightest convex extension is NP-hard. However, by applying our characterization to every function in an additive decomposition of the objective function, we obtain a class of looser convex extensions that can be computed efficiently. For some decompositions, common loss and regularization functions, we derive a closed form.

1. Introduction

We study an optimization problem: Given a finite set $S \neq \emptyset$ whose elements are to be labeled as 0 or 1, a non-empty set $Y \subseteq \{0, 1\}^S$ of *feasible labelings*, $x : S \rightarrow \mathbb{R}^m$ with $m \in \mathbb{N}$, called a *feature matrix*, $l : \mathbb{R} \times [0, 1] \rightarrow \mathbb{R}_0^+$ with $l(\cdot, 0)$ convex, $l(\cdot, 1)$ convex, $l(r, 1) \rightarrow 0$ as $r \rightarrow \infty$ and $l(-r, 0) \rightarrow 0$ as $r \rightarrow \infty$, called a *loss function*, $\Theta \subseteq \mathbb{R}^m$ convex, called the set of *feasible parameters*, $\omega : \Theta \rightarrow \mathbb{R}_0^+$ convex, called a *regularization function*, and $C \in \mathbb{R}_0^+$, called a *regularization constant*, we consider the optimization problem

$$\inf_{(\theta, y) \in \Theta \times Y} \varphi(\theta, y) \quad (1)$$

with

$$\varphi(\theta, y) := \omega(\theta) + \frac{C}{|S|} \sum_{s \in S} l_s(\theta, y_s) \quad (2)$$

$$l_s(\theta, y_s) := l(\langle x_s, \theta \rangle, y_s) . \quad (3)$$

A minimizer $(\hat{\theta}, \hat{y})$, if it exists, defines a *classifier* $c : \mathbb{R}^m \rightarrow \{0, 1\} : x \mapsto \frac{1}{2}(1 + \text{sgn} \langle \hat{\theta}, x \rangle)$ and a feasible labeling $\hat{y} \in Y$. The optimization problem (1) is a remarkably general abstraction of learning. On the one hand, it generalizes supervised, semi-supervised and unsupervised learning:

- If the labeling y is fixed by $|Y| = 1$ to precisely one feasible labeling, (1) specializes to *regularized empirical risk minimization with fixed labels* and is called *supervised*.
- If Y fixes the label of at least one but not all elements of S , (1) is called *semi-supervised*.
- If Y constrains the joint labelings of S without fixing the label of any single element of S , (1) is called *unsupervised*. For example, consider $Y = \{y \in \{0, 1\}^S \mid \sum_{s \in S} y_s = \lfloor |S|/2 \rfloor\}$.

On the other hand, the optimization problem (1) generalizes classification, clustering and ranking:

- If $S = A \times B$ and Y is the set of characteristic functions of *maps* from A to B , (1) is an abstraction of *multi-label classification*, as discussed, for instance, by [Joachims \(1999, 2003\)](#); [Chapelle and Zien \(2005\)](#); [Xu and Schuurmans \(2005\)](#); [Chapelle et al. \(2006b,a, 2008\)](#).
- If $S = A \times A$ and Y is the set of characteristic functions of *equivalence relations* on A , (1) is an abstraction of *clustering*, as discussed by [Finley and Joachims \(2005\)](#); [Xu et al. \(2005\)](#). For fixed parameters θ , it specializes to the NP-hard minimum cost clique partition problem ([Grötschel and Wakabayashi, 1989](#); [Chopra and Rao, 1993](#)) that is also known as correlation clustering ([Bansal et al., 2004](#); [Demaine et al., 2006](#)).
- If $S = A \times A$ and Y is the set of characteristic functions of *linear orders* on A , (1) is an abstraction of *ranking*. For fixed parameters θ , it specializes to the NP-hard linear ordering problem ([Martí and Reinelt, 2011](#)).

The set Y of feasible labelings, a subset of the vertices of the unit hypercube $[0, 1]^S$, is a non-convex subset of \mathbb{R}^S iff $2 \leq |Y|$. Typically, one considers a relaxation $y \in P$ of the constraint $y \in Y$ with P a convex polytope such that $\text{conv } Y \subseteq P \subseteq [0, 1]^S$ and $P \cap \{0, 1\}^S = Y$. In practice, one considers a polytope that is described as an intersection of half-spaces, i.e., by $n \in \mathbb{N}$, $A \in \mathbb{R}^{n \times S}$ and $b \in \mathbb{R}^n$ such that $P = \{y \in \mathbb{R}^S \mid Ay \leq b\}$. Also typically, the set $\Theta \subseteq \mathbb{R}^m$ of feasible parameters is a convex polyhedron and is described also as an intersection of half-spaces, i.e., by $n' \in \mathbb{N}$, $A' \in \mathbb{R}^{n' \times m}$ and $b' \in \mathbb{R}^{n'}$ such that $\Theta = \{\theta \in \mathbb{R}^m \mid A'\theta \leq b'\}$. Hence, the optimization problem (1) assumes the form of a mixed integer program (MIP):

$$\inf_{(\theta, y) \in \mathbb{R}^m \times [0, 1]^S} \varphi(\theta, y) \quad (4)$$

$$\text{subject to } A'\theta \leq b' \quad (5)$$

$$Ay \leq b \quad (6)$$

$$y \in \{0, 1\}^S \quad (7)$$

For *convex* loss functions l_s such as the squared difference loss (Tab. 1), the objective function φ is convex on the domain $\mathbb{R}^m \times [0, 1]^S$. Thus, the continuous relaxation (4)–(6) of the problem (4)–(7) is a convex problem. Its solutions $(\hat{\theta}', \hat{y}')$, although possibly fractional in the coordinates of y' , can inform a search for feasible solutions of (4)–(7) with certificates ([Chapelle et al., 2006b, 2008](#); [Bojanowski et al., 2013](#)). See also [Bonami et al. \(2012\)](#) for a recent survey of convex mixed-integer non-linear programming. For *non-convex* loss functions l_s such as the logistic loss, the Hinge loss and the squared Hinge loss (Tab. 1), φ is non-convex on the domain $\mathbb{R}^m \times [0, 1]^S$. In this case, (4)–(7) is resistant to standard optimization techniques. See [Tawarmalani and Sahinidis \(2004\)](#); [Lee and Leyffer \(2011\)](#); [Belotti et al. \(2013\)](#) for an overview of non-convex mixed-integer non-linear programming.

Table 1: Loss functions

Loss	Form of $l_s(\theta, y_s)$	Function $l_s : \mathbb{R}^m \times [0, 1] \rightarrow \mathbb{R}_0^+$
Squared difference	$(\langle \theta, x_s \rangle - y_s)^2$	convex
Logistic	$\log(1 + \exp(-(2y_s - 1)\langle \theta, x_s \rangle))$	non-convex
Hinge	$\max\{0, 1 - (2y_s - 1)\langle \theta, x_s \rangle\}$	non-convex
Squared Hinge	$\max\{0, 1 - (2y_s - 1)\langle \theta, x_s \rangle\}^2$	non-convex

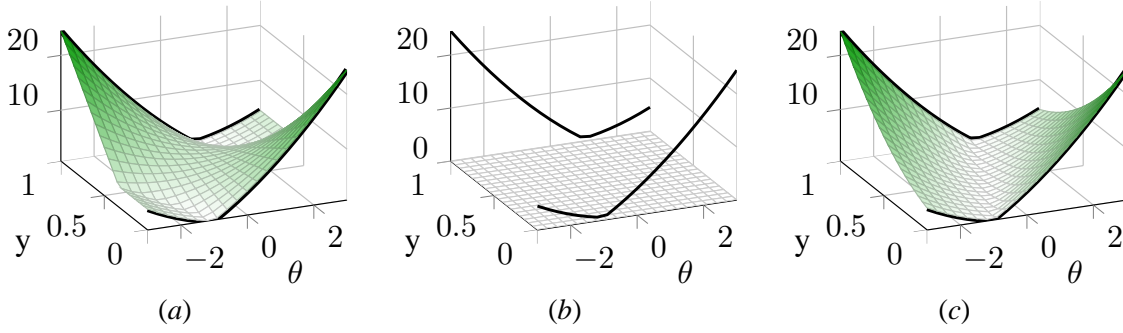


Figure 1: Depicted above in (a) is the non-convex objective function φ of the optimization problem (1) for $Y = \{0, 1\}$, $\Theta = \mathbb{R}$, the Hinge loss (Tab. 1) and $\omega(\cdot) = \|\cdot\|_2^2$. Its restriction ϕ to the feasible set $\Theta \times \{0, 1\}$ is depicted in black. As the goal is to minimize φ over the feasible set, one can replace the values of φ for $y \in (0, 1)$ without affecting the solution, for instance, by zero, as depicted in (b). In this paper, we characterize the tightest convex extension of ϕ to $\Theta \times \text{conv } Y$, which is depicted in (c).

1.1. Contribution

We construct, for the MIP (4)–(7) whose objective function is non-convex, MIPs with the same solutions whose objective functions are convex. Our approach is illustrated in Fig. 1 and is summarized below.

In Section 3, we consider the restriction ϕ of φ to the feasible set $\Theta \times Y$ and characterize the tightest convex extension ϕ^{**} of ϕ to $\Theta \times \text{conv } Y$. This tightest convex extension ϕ^{**} is mostly of theoretical interest as computing its values is NP-hard.

In Section 4, we consider a decomposition of the function ϕ into a sum of functions. By applying our characterization of tightest convex extensions to every function in this sum, we construct a convex extension ϕ' of ϕ to $\Theta \times [0, 1]^S$ which is not generally tight but whose values can be computed efficiently. For common loss and regularization functions, we derive a closed form.

For every convex extension ϕ' we construct, including ϕ^{**} , the MIP

$$\inf_{(\theta, y) \in \mathbb{R}^m \times \mathbb{R}^S} \phi'(\theta, y) \quad (8)$$

$$\text{subject to } A'\theta \leq b' \quad (9)$$

$$Ay \leq b \quad (10)$$

$$y \in \{0, 1\}^S \quad (11)$$

has the same solutions as (4)–(7). Like (4)–(7), it is NP-hard, due to the integrality constraint (11). Unlike (4)–(7), its objective function and polyhedral relaxation (8)–(10) are convex. Thus, unlike (4)–(7), it is accessible to a wide range of standard optimization techniques.

2. Related Work

2.1. Convex Extensions

For large classes of univariate and bivariate functions, tightest convex extensions have been characterized by [Tawarmalani et al. \(2013\)](#) and [Locatelli \(2014\)](#). Convex envelopes of multivariate functions that are convex in all but one variable have been characterized by [Jach et al. \(2008\)](#). For functions of the form $f(x, y) = g(x)h(y)$ and with g and h having additional properties, e.g., g being component-wise concave and submodular, and h being univariate convex, tightest convex extensions have been characterized by [Khajavirad and Sahinidis \(2012, 2013\)](#). For functions $f : A \times B \rightarrow \mathbb{R}$ with $A, B \subseteq \mathbb{R}^n$ and $f(a, \cdot)$ being either convex or concave and $f(\cdot, b)$ being either convex or concave for any $a \in A$ and $b \in B$, tightest convex extensions have been characterized by [Ballerstein \(2013\)](#). Tightest convex extensions of pseudo-Boolean functions $f : \{0, 1\}^n \rightarrow \mathbb{R}$ are known as convex closures ([Bach, 2013](#)). Convex closures of submodular functions are Lovász extensions.

The characterization of tightest convex extensions of functions $f : \Theta \times Y \rightarrow \mathbb{R}$ with $f(\cdot, y)$ convex for all $y \in Y$ that we establish is consistent with results of [Jach et al. \(2008\)](#) for functions $f : \mathbb{R}^n \times \{0, 1\} \rightarrow \mathbb{R}$. It extends some results of [Jach et al. \(2008\)](#) to non-differentiable $f(\cdot, 0)$ and $f(\cdot, 1)$.

2.2. Regularized Empirical Risk Minimization with Constrained Labels

Regularized empirical risk minimization with constrained labels has been studied intensively in the special case of semi-supervised learning for 01-classification. Algorithms that find feasible solutions efficiently are due to [Joachims \(1999, 2003\)](#); [Chapelle and Zien \(2005\)](#); [Chapelle et al. \(2006a,b\)](#); [Sindhwani et al. \(2006\)](#). A branch-and-bound algorithm that solves the problem to optimality was suggested by [Vapnik and Chervonenkis \(1974\)](#) and has been implemented and applied to data by [Chapelle et al. \(2006b, 2008\)](#), with the result that optimal solutions generalize better typically than feasible solutions found by approximate algorithms.

An approach to the problem by convex optimization, specifically, by a semi-definite relaxation of the dual problem, was proposed by [Bie and Cristianini \(2006\)](#). Similar relaxations have been studied in the context of semi-supervised learning for multi-label classification ([Xu and Schuurmans, 2005](#); [Guo and Schuurmans, 2011](#)), correlation clustering ([Xu et al., 2005](#); [Zhang et al., 2009](#)) and latent variable estimation ([Guo and Schuurmans, 2008](#)). For maximum margin clustering, a convex relaxation tighter than the SDP relaxation is constructed by [Li et al. \(2009\)](#). For multi-label classification with a softmax loss function, a tight SDP relaxation is proposed by [Joulin and Bach \(2012\)](#).

3. Tightest Convex Extensions

In this section, we consider the restriction ϕ of φ to the feasible set $\Theta \times Y$, i.e., the function

$$\phi : \Theta \times Y \rightarrow \mathbb{R}_0^+ : (\theta, y) \mapsto \varphi(\theta, y) . \quad (12)$$

We characterize the tightest convex extension ϕ^{**} of ϕ to $\Theta \times \text{conv } Y$ in Theorem 3.

Definition 1 (*Tawarmalani and Sahinidis, 2002*) For any $n \in \mathbb{N}$, any $A \subseteq \mathbb{R}^n$ and any $\phi : A \rightarrow \mathbb{R}$, a function $\phi' : \text{conv } A \rightarrow \mathbb{R}$ is called a *convex extension* of ϕ iff ϕ' is convex and $\forall a \in A : \phi'(a) = \phi(a)$. Moreover, a function $\phi^{**} : \text{conv } A \rightarrow \mathbb{R}$ is called the *tightest convex extension* of ϕ iff ϕ^{**} is a convex extension of ϕ and, for every convex extension ϕ' of ϕ and for all $a \in \text{conv } A$: $\phi'(a) \leq \phi^{**}(a)$.

Lemma 2 A (tightest) convex extension ϕ^{**} of ϕ exists.

Theorem 3 For every finite $S \neq \emptyset$, every $Y \subseteq \{0, 1\}^S$ with $|Y| > |S|$, every $m \in \mathbb{N}$, every convex $\Theta \subseteq \mathbb{R}^m$ and every $\phi : \Theta \times Y \rightarrow \mathbb{R}_0^+$ such that $\phi(\cdot, y)$ is convex for every $y \in Y$, the tightest convex extension $\phi^{**} : \Theta \times \text{conv } Y \rightarrow \mathbb{R}_0^+$ of ϕ is such that for all $(\theta, y) \in \Theta \times \text{conv } Y$:

$$\phi^{**}(\theta, y) = \min_{Y' \in \mathcal{Y}(y)} \inf_{\theta' : Y' \rightarrow \Theta} \left\{ \sum_{y' \in Y'} \lambda_{yY'}(y') \phi(\theta'(y'), y') \mid \sum_{y' \in Y'} \lambda_{yY'}(y') \theta'(y') = \theta \right\} \quad (13)$$

where

$$\mathcal{Y}(y) := \left\{ Y' \in \binom{Y}{|S|+1} \mid y \in \text{conv } Y' \right\} \quad (14)$$

is the set of $(|S| + 1)$ -elementary subsets Y' of Y having y in their convex hull, and, for every $y \in \text{conv } Y$ and every $Y' \in \mathcal{Y}(y)$: $\lambda_{yY'} : Y' \rightarrow \mathbb{R}_0^+$ are the coefficients in the convex combination of y in Y' , i.e.

$$\sum_{y' \in Y'} \lambda_{yY'}(y') y' = y \quad (15)$$

$$\sum_{y' \in Y'} \lambda_{yY'}(y') = 1 . \quad (16)$$

Remarks are in order:

- $|\mathcal{Y}(y)|$ can be strongly exponential in $|S|$. This is expected, given that the complexity of computing the value of a convex extension is NP-hard.
- Given a polynomial-time oracle for the outer minimization in (13), the tightest convex extension can be computed in polynomial time.
- Conceivable is a polynomial-time oracle for constraining $\mathcal{Y}(y)$ to a strict subset without compromising optimality in (13).
- An upper bound on the tightest convex extension can be obtained by considering any subset of $\mathcal{Y}(y)$.

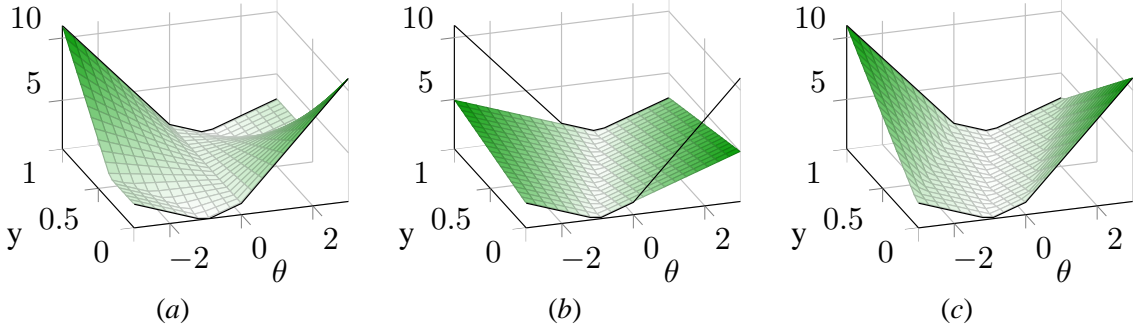


Figure 2: Depicted above in (a) is the non-convex objective function φ of the optimization problem (1) for $Y = \{0, 1\}$, $\Theta = \mathbb{R}$, the Hinge loss (Tab. 1) and $\omega(\cdot) = \|\cdot\|_1$. Its restriction ϕ to $\Theta \times \{0, 1\}$ is depicted in black. Depicted in (b) is the tightest convex extension of ϕ to $\Theta \times [0, 1]$. Depicted in (c) is the tightest convex extension of ϕ to $[-b, b] \times [0, 1]$, for $b \in \mathbb{R}_0^+$. It can be seen that, for bounded θ , the tightest convex extension is continuous.

4. Efficient Convex Extensions

In this section, we characterize, for common loss and regularization functions, convex extensions ϕ' of ϕ that are not necessarily tight but can be computed efficiently in general. The construction is in two steps:

Firstly, we consider an additive decomposition of ϕ . Specifically, we consider a convex function $c : \Theta \rightarrow \mathbb{R}_0^+$ and, for every $s \in S$, a function $d_s : \Theta \times \{0, 1\} \rightarrow \mathbb{R}_0^+$ such that $d_s(\cdot, 0)$ and $d_s(\cdot, 1)$ are convex. These functions are chosen such that, for all $(\theta, y) \in \Theta \times Y$:

$$\phi(\theta, y) = c(\theta) + \frac{1}{|S|} \sum_{s \in S} d_s(\theta, y_s) . \quad (17)$$

One example is given by $c := \omega$ and, for every $s \in S$, $d_s := Cl_s$. Another example is given by $c := 0$ and, for every $s \in S$, every $\theta \in \Theta$ and every $y_s \in \{0, 1\}$: $d_s(\theta, y_s) := \omega(\theta) + Cl_s(\theta, y_s)$.

Secondly, we characterize, for each d_s , its tightest convex extension $d_s^{**} : \Theta \times [0, 1] \rightarrow \mathbb{R}$, by a specialization of Theorem 3 stated as Corollary 4. A convex extension ϕ' of ϕ to $\Theta \times [0, 1]^S$ is then given by

$$\phi' : \Theta \times [0, 1]^S \rightarrow \mathbb{R}_0^+ : (\theta, y) \mapsto c(\theta) + \frac{1}{|S|} \sum_{s \in S} d_s^{**}(\theta, y_s) . \quad (18)$$

Corollary 4 *For every $d : \Theta \times \{0, 1\} \rightarrow \mathbb{R}_0^+$ such that $d_0(\cdot) := d(\cdot, 0)$ and $d_1(\cdot) := d(\cdot, 1)$ are convex, the tightest convex extension $d^{**} : \Theta \times [0, 1] \rightarrow \mathbb{R}_0^+$ of d is such that for all $(\theta, y) \in \Theta \times Y$:*

$$d^{**}(\theta, y) = \begin{cases} d(\theta, y) & \text{if } y \in \{0, 1\} \\ \Psi(\theta, y) & \text{if } y \in (0, 1) \end{cases} \quad (19)$$

with

$$\Psi(\theta, y) = \inf_{\theta^0, \theta^1 \in \Theta} \{ (1-y)d_0(\theta^0) + yd_1(\theta^1) \mid (1-y)\theta^0 + y\theta^1 = \theta \} . \quad (20)$$

The solutions of the optimization problem (20) are characterized in Lemma 5. Subgradients are given in Lemma 6.

Lemma 5 *For every solution $(\hat{\theta}^0, \hat{\theta}^1) \in \Theta^2$ of (20), there exists a $G \neq \emptyset$ such that, for $\xi_{\theta,y} : \Theta \rightarrow \Theta : t \mapsto (\theta - (1-y)t)/y$:*

$$(\delta d_0)(\hat{\theta}^0) \cap (\delta d_1)(\xi_{\theta,y}(\hat{\theta}^0)) = G \quad (21)$$

$$(\delta d_0)(\xi_{\theta,1-y}(\hat{\theta}^1)) \cap (\delta d_1)(\hat{\theta}^1) = G . \quad (22)$$

Lemma 6 *If a solution $(\hat{\theta}^0, \hat{\theta}^1) \in \Theta^2$ of (20) exists, then $\begin{pmatrix} v \\ w \end{pmatrix} \in (\delta d^{**})(\theta, y)$ iff $v \in G$ with G defined equivalently in (21) and (22) and $w = v^T \hat{\theta}^0 - v^T \hat{\theta}^1 + d_1(\hat{\theta}^1) - d_0(\hat{\theta}^0)$. Otherwise, $y \in \{0, 1\}$ and:*

$$y = 0 \quad \Rightarrow \quad \forall v \in (\delta d(\cdot, 0))(\theta) : \begin{pmatrix} v \\ \infty \end{pmatrix} \in (\delta d^{**})(\theta, y) \quad (23)$$

$$y = 1 \quad \Rightarrow \quad \forall v \in (\delta d(\cdot, 1))(\theta) : \begin{pmatrix} v \\ -\infty \end{pmatrix} \in (\delta d^{**})(\theta, y) . \quad (24)$$

We proceed as follows: In Section 4.1, we consider two decompositions of the class (17) for which the tightest convex extension of any d_s is easy to characterize but the resulting convex extension of ϕ is rather loose. In Sections 4.2 and 4.3, we consider decompositions of the class (17) with $c = 0$. These yield the tightest convex extension of ϕ of any decomposition of the class (17). For any combination of the logistic loss, the Hinge loss and the squared Hinge loss (Tab. 1) with either L1 regularization $\omega(\cdot) = \|\cdot\|_1$ or L2 regularization $\omega(\cdot) = \|\cdot\|_2^2$, we characterize the convex extension explicitly and, in some cases, in closed form. Examples of all combinations are depicted in Fig. 3.

4.1. Instructive Examples

The first convex extension we characterize is for the decomposition (17) with $c := \omega$ and $\forall s \in S : d_s := Cl_s$.

Corollary 7 *For any $d : \Theta \times \{0, 1\} \rightarrow \mathbb{R}_0^+$ such that $d_0(\cdot) := d(\cdot, 0)$ and $d_1(\cdot) := d(\cdot, 1)$ are convex and for which $d_0(-r) \rightarrow 0$ and $d_1(r) \rightarrow 0$ as $r \rightarrow \infty$, the convex extension $d^{**} : \Theta \times [0, 1] \rightarrow \mathbb{R}$ of d has the form*

$$d'(\theta, y) = \begin{cases} d(\theta, y) & \text{if } y \in \{0, 1\} \\ 0 & \text{if } y \in (0, 1) \end{cases} . \quad (25)$$

The second convex extension we characterize is for the logistic loss $l_s(\theta, y) = -\langle x, \theta \rangle y + \log(1 + e^{\langle x, \theta \rangle})$, for $\omega(\cdot) = \|\cdot\|_2^2$ and for the decomposition (17) such that, for every $s \in S$, $d_s(\theta, y) := \|\theta\|_2^2 - C\langle x, \theta \rangle y$.

Corollary 8 *The tightest convex extension $d^{**} : \Theta \times [0, 1] \rightarrow \mathbb{R}_0^+$ of $d : \Theta \times \{0, 1\} \rightarrow \mathbb{R}_0^+$ with $d(\theta, y) = \|\theta\|_2^2 - C\langle x, \theta \rangle y$ has the form $d^{**}(\theta, y) = \|\theta - y\frac{C}{2}x\|_2^2 - y\|\frac{C}{2}x\|_2^2$.*

4.2. L2 Regularization

We now consider $\omega(\cdot) = \frac{1}{2} \|\cdot\|_2^2$ and decompositions (17) such that, for every $s \in S$: $d_s(\theta, y) = \omega(\theta) + C l_s(\theta, y)$.

Corollary 9 *The tightest convex extension $d^{**} : \Theta \times [0, 1] \rightarrow \mathbb{R}_0^+$ of $d : \Theta \times \{0, 1\} \rightarrow \mathbb{R}_0^+$ with $d(\theta, y) = \frac{1}{2} \|\theta\|_2^2 + Cl(\langle x, \theta \rangle, y)$ is given by (19) and (20). Moreover, the solution of (20) is given by $\hat{\theta}^0 = \theta - yCxz$ with*

$$z \in (\delta l_0)(x^T(\theta - yCxz)) - (\delta l_1)(x^T(\theta + (1 - y)Cxz)) \subseteq \mathbb{R}. \quad (26)$$

Although this characterization is not a closed form, values of d^{**} can be computed efficiently using the bisection method. For specific loss functions, closed forms are derived below.

Corollary 10 *The tightest convex extension $d^{**} : \Theta \times [0, 1] \rightarrow \mathbb{R}_0^+$ of $d : \Theta \times \{0, 1\} \rightarrow \mathbb{R}_0^+$ with $d(\theta, y) = \frac{1}{2} \|\theta\|_2^2 + Cl(\langle x, \theta \rangle, y)$ and $l : \mathbb{R} \times \{0, 1\} \rightarrow \mathbb{R}_0^+$ of the form*

$$l(r, y) = (C_0(1 - y) + C_1y) \max\{0, 1 - (2y - 1)r\} \quad (27)$$

where $C_0, C_1 \in \mathbb{R}_+$ define weights on the two values of y , is given by Corollary 9. Moreover, every z satisfying (26) holds

$$z \in \left\{ 0, C_0, C_1, C_0 + C_1, \frac{1 + x^T \theta}{yC x^T x}, \frac{1 - x^T \theta}{(1 - y)C x^T x} \right\}. \quad (28)$$

Corollary 11 *The tightest convex extension $d^{**} : \Theta \times [0, 1] \rightarrow \mathbb{R}_0^+$ of $d : \Theta \times \{0, 1\} \rightarrow \mathbb{R}_0^+$ with $d(\theta, y) = \frac{1}{2} \|\theta\|_2^2 + Cl(\langle x, \theta \rangle, y)$ and $l : \mathbb{R} \times \{0, 1\} \rightarrow \mathbb{R}_0^+$ of the form*

$$l(r, y) = \frac{C_0(1 - y) + C_1y}{2} (\max\{0, 1 - (2y - 1)r\})^2 \quad (29)$$

where $C_0, C_1 \in \mathbb{R}_+$ define weights on the two values of y , is given by Corollary 9. Moreover, every z satisfying (26) holds

$$z \in \left\{ 0, \frac{C_0 + C_0 x^T \theta}{1 + C_0 y C x^T x}, \frac{C_1 - C_1 x^T \theta}{1 + C_1(1 - y)C x^T x}, \frac{C_0 + C_1 + (C_0 - C_1)x^T \theta}{1 + (C_0 y + C_1(1 - y))C x^T x} \right\}. \quad (30)$$

4.3. L1 regularization

We now consider $\omega(\cdot) = \|\cdot\|_1$ and decompositions (17) such that, for every $s \in S$: $d_s(\theta, y) = \omega(\theta) + C l_s(\theta, y)$. We focus on a special case where θ is bounded. This is necessary in order for the convex extension to be continuous; see Fig. 2.

Corollary 12 *For $b, t \in (\mathbb{R} \cup \{-\infty, \infty\})^m$ and $\Theta = \{\theta \in \mathbb{R}^m : b \leq \theta \leq t\}$, the tightest convex extension $d^{**} : \Theta \times [0, 1] \rightarrow \mathbb{R}_0^+$ of $d : \Theta \times \{0, 1\} \rightarrow \mathbb{R}_0^+$ with $d(\theta, y) = \|\theta\|_1 + Cl(\langle x, \theta \rangle, y)$ is given by (19) and (20). Moreover, the solution of (20) is given by*

$$\hat{\theta}^0 = \begin{cases} \theta' & \text{if } \exists r \in a(x^T \theta') : \|rCx\|_\infty \leq 2 \\ \text{aux}(\theta', x, a, b, t) & \text{otherwise} \end{cases} \quad (31)$$

with $a : \mathbb{R} \rightarrow 2^{\mathbb{R}} : p \mapsto (\delta l_0)(p) - (\delta l_1)((x^T \theta - (1 - y)p)/y)$ and

$$\forall i \in \{1, \dots, m\} : \quad \theta'_i = \begin{cases} \min_{r \in [b'_i, t'_i]} |r| & \text{if } \theta_i > 0 \Leftrightarrow x_i > 0 \\ \min_{r \in [b'_i, t'_i]} \left| \frac{\theta_i}{(1 - y)} - r \right| & \text{otherwise} \end{cases}. \quad (32)$$

The function “aux” is defined below in terms of Alg. 1. At its core, this algorithm solves, for fixed $k \in [m]$ and fixed $V \in \Theta$, the equation (33) for the unknown $z \in \mathbb{R}$. For specific loss functions, closed forms are derived in Corollaries 13 and 14.

$$|a(x^T V - zx_k) Cx_k| = 2 \quad (33)$$

Corollary 13 *The tightest convex extension $d^{**} : \Theta \times [0, 1] \rightarrow \mathbb{R}_0^+$ of $d : \Theta \times \{0, 1\} \rightarrow \mathbb{R}_0^+$ with $d(\theta, y) = \|\theta\|_1 + Cl(\langle x, \theta \rangle, y)$ and $l : \mathbb{R} \times \{0, 1\} \rightarrow \mathbb{R}_0^+$ of the form*

$$l(r, y) = (C_0(1 - y) + C_1 y) \max\{0, 1 - (2y - 1)r\} \quad (34)$$

where $C_0, C_1 \in \mathbb{R}_+$ define weights on the two values of y , is given by Corollary 12. Moreover, every solution $z \in \mathbb{R}$ of (33) holds

$$z \in \left\{ \frac{1 + x^T V}{x_k^2}, \frac{y + x^T(\theta - (1 - y)V)}{(1 - y)x_k^2} \right\}. \quad (35)$$

Corollary 14 *The tightest convex extension $d^{**} : \Theta \times [0, 1] \rightarrow \mathbb{R}_0^+$ of $d : \Theta \times \{0, 1\} \rightarrow \mathbb{R}_0^+$ with $d(\theta, y) = \|\theta\|_1 + Cl(\langle x, \theta \rangle, y)$ and $l : \mathbb{R} \times \{0, 1\} \rightarrow \mathbb{R}_0^+$ of the form*

$$l(r, y) = \frac{C_0(1 - y) + C_1 y}{2} (\max\{0, 1 - (2y - 1)r\})^2 \quad (36)$$

where $C_0, C_1 \in \mathbb{R}_+$ define weights on the two values of y , is given by Corollary 12. Moreover, every solution $z \in \mathbb{R}$ of (33) holds (37) with $v_0 := x^T V$ and $v_1 := -x^T \xi_{\theta, y}(V)$.

$$z \in \left\{ \frac{1 + v_0 - 2(C|x_k|C_0)^{-1}}{x_k^2}, \frac{1 + v_1 - 2(C|x_k|C_1)^{-1}}{x_k^2}, \frac{y(C_0(1 + v_0) + C_1(1 + v_1) - 2(C|x_k|)^{-1})}{(yC_0 + (1 - y)C_1)x_k^2} \right\} \quad (37)$$

5. Conclusion

We have characterized convex extensions, including the tightest convex extension, of functions $f : \Theta \times Y \rightarrow \mathbb{R}_0^+$ with $\Theta \subseteq \mathbb{R}^m$ convex, $Y \subseteq \{0, 1\}^n$ and $f(\cdot, y)$ convex for every $y \in \{0, 1\}^n$. This has allowed us to state regularized empirical risk minimization with constrained labels as a mixed integer program whose objective function is convex. Convex extensions that strike a practical balance between tightness and computational complexity are a topic of future work.

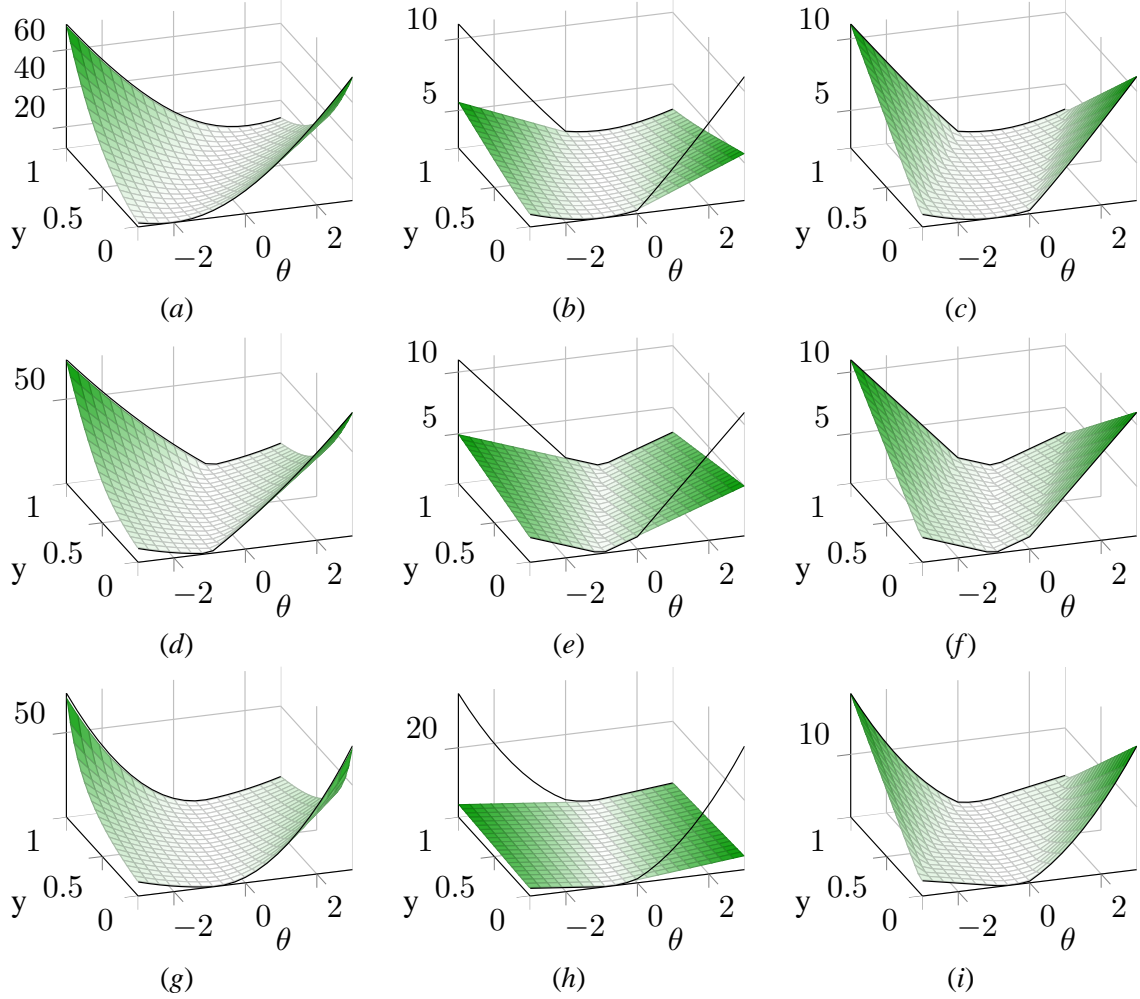


Figure 3: Depicted above are tightest convex extensions of the logistic loss (first row), the Hinge loss (second row) and the squared Hinge loss (third row), in conjunction with L2 regularization (first column), L1 regularization (second column) and L1 regularization with θ constrained to $[-3.1, 3.1]$ (third column). Values for $y \in \{0, 1\}$ are depicted in black. Note that the convex extensions of L1-regularized loss functions for unbounded θ are discontinuous. Parameters for these examples are $x = 1$ and $\mathfrak{3}(a)$: $C = 16$, $\mathfrak{3}(b)$: $C = 5$, $\mathfrak{3}(c)$: $C = 5$, $\mathfrak{3}(d)$: $C = 16$, $\mathfrak{3}(e)$: $C = 5$, $\mathfrak{3}(f)$: $C = 5$, $\mathfrak{3}(g)$: $C = 4$, $\mathfrak{3}(h)$: $C = 4$. $\mathfrak{3}(i)$: $C = 4$.

Input: $\theta', x \in \mathbb{R}^n, a : \mathbb{R} \rightarrow 2^{\mathbb{R}}, C \in \mathbb{R}_0^+, b, t \in (\mathbb{R} \cup \{-\infty, \infty\})^n$
Output: $V \in \Theta$
 $V := \theta'$
 $\forall i \in [n] : b'_i := \max\{b_i, (\xi_{\theta, 1-y}(t))_i\}$
 $\forall i \in [n] : t'_i := \min\{t_i, (\xi_{\theta, 1-y}(b))_i\}$
 $I \in \mathbb{N}^n$ such that $|x_{I_1}| \geq |x_{I_2}| \geq \dots \geq |x_{I_n}|$
for $j = 1 \dots n$ **do**
 if $\exists r \in a(x^T V) : \|rCx\|_{\infty} \leq 2$ **then**
 return V
 end
 $i := I_j$
 if $x_i > 0$ **then**
 $V_i := b'_i$
 else
 $V_i := t'_i$
 end
 if $\exists r \in a(x^T V) : \|rCx\|_{\infty} \leq 2$ **then**
 $V_i := V_i - zx_k$ with $z \in \mathbb{R}$ such that $|a(x^T V - zx_k)Cx_k| = 2$
 return V
 end
end
return V

Algorithm 1: Computation of the function “aux”

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