1 Context

Regularization-based approaches for injecting constraints in Machine Learning (ML) were introduced (see e.g. [3]) to improve a predictive model via expert knowledge. Given the recent interest in ethical and trustworthy AI, however, several works are resorting to these approaches for enforcing desired properties over a ML model (e.g. fairness [1, 5, 2]). Regularized approaches for constraint injection solve, in an exact or approximate fashion, a problem in the form:

$$\arg\min_{w \in W} \{L(y) + \lambda^\top C(y)\} \quad \text{with: } y = f(\mathbf{x}; w)$$

where $L$ is a loss function and $f$ is the model to be trained, with parameter vector $w$ from a parameter space $W$. We use $f(\mathbf{x}; w)$ to refer to the model output for the whole training set $\mathbf{x}$. The regularization function $C$ denotes a vector of (non-negative) constraint violation indices for $m$ constraints, while $\lambda \geq 0$ is a vector of weights (or multipliers).

As an example, in a regression problem we may desire a specific output ordering for two input vectors in the training set. A viable regularizer may be:

$$C(y) = \max(0, y_i - y_j)$$

the term is zero iff the constraint $y_i \leq y_j$ is satisfied. For obtaining balanced predictions in a binary classification problem, we may use instead:

$$C(y) = \left| \sum_{i=1}^{n} y_i - \frac{n}{2} \right|$$

where $y_i$ is the binary output associated to one of the two classes. If $n$ is even, the term is 0 for perfectly balanced classifications.

When regularized methods are used to enforce constraints, a typical approach consists in adjusting the $\lambda$ vector until a suitable compromise between accuracy and constraint satisfaction is reached (e.g. a discrimination index becomes sufficiently low). This approach enables the use of traditional training algorithms, at the cost of having to search over the space of possible multipliers.

Though the method is known to work well in many practical cases, the process has been subject to little general analysis. With this note, we aim to make a preliminary step in this direction, providing a more systematic overview of the strengths and (in particular) potential weaknesses of this class of approaches.
With some abuse of notation, we wish to understand the viability of solving PC indirectly, by adjusting the PR formulation and the following constrained training problem:

\[ \text{PC}(\lambda) : \text{arg min}_{w \in W} \{ L(w) \mid C(w) \leq \theta \} \]

where \( \theta \) is a vector of thresholds for the constraint violation indices. In ethical or trustworthy AI applications, PC will be the most natural problem formulation.

We wish to understand the viability of solving PC indirectly, by adjusting the \( \lambda \) vector and solving the unconstrained problem PR, as depicted in Algorithm 1; line 2 refers to some kind of search over the multiplier space. Ideally, the algorithm should be equivalent to solving the PC formulation directly. For this to be true, solving PR(\( \lambda \)) should have a chance to yield assignments that are optimal for the constrained problem. Moreover, an optimum of PC(\( \theta \)) should always be attainable in this fashion. Additional properties may enable more efficient search. In the note, we will characterize Algorithm 1 to the best of our abilities.

### Regularized and Constrained Optima

The relation between the PR and PC formulations are tied to the properties of their optimal solutions. An optimal PC solution \( w^*_p \) satisfies:

\[ \text{opt}_c(w^*, \theta) : L(w) \geq L(w^*) \quad \forall w \in W \mid C(w) \leq \theta \]

while for an optimal solution \( w^*_r \) of PR with multipliers \( \lambda \) we have:

\[ \text{opt}_r(w^*, \lambda) : L(w) + \lambda^\top C(w) \geq L(w^*) + \lambda^\top C(w^*) \quad \forall w \in W \]

The definitions apply also to local optima, by swapping \( W \) with some neighborhood of \( w^*_p \) and \( w^*_r \). We can now provide the following result:

**Theorem 1** an optimal solution \( w^* \) for PR is also optimal for PC, for a threshold equal to \( C(w^*) \):

\[ \text{opt}_r(w^*, \lambda) \Rightarrow \text{opt}_c(w^*, C(w^*)) \]

**Proof (by contradiction)** Let us assume that \( w^* \) is an optimal solution for PR but not optimal for PC, i.e. that there is a feasible \( w' \in W \) such that:

\[ L(w') < L(w^*) \]

Since \( w^* \) is optimal for PR, we have that:

\[ L(w') \geq L(w^*) + \lambda^\top (C(w^*) - C(w')) \]

Since \( w' \) is feasible for \( \theta = C(w^*) \), we have that its violation vector cannot be greater than that of \( w^* \). Formally, we have that \( C(w') \leq C(w^*) \), or equivalently \( C(w^*) - C(w') \geq 0 \). Therefore Equation (10) contradicts Equation (9), thus proving the original point. The same reasoning applies to local optima.

Theorem 1 shows that solving PR(\( \lambda \)) always results in an optimum for the constrained formulation, albeit for threshold \( \theta = C(w^*) \) that cannot be a priori chosen. The statement is true even for non-convex loss, regularizer, and model structure. This is a simple, but powerful result, which provides a strong motivation for Algorithm 1.
The proof is omitted due to lack of space. When monotonicity holds, searching over the multiplier space in Algorithm 1, which constraint the violation is higher enforces a lower bound. Additionally, it may happen that different constrained optima are associated to the same multiplier, can be considerably simpler (e.g. binary search for a single multiplier, or sub-gradient descent in general [4]).

Further issues arise (even for global optimality) when the regularized problem PR(λ) has multiple equivalent optima. In the fully convex case, this may happen if the multiplier values cause the presence of plateaus (see Figure 1A, where λ_j = 1). In the (more practically relevant) non-convex case, there may be separate optima with the same value for the regularized loss, but different trade-offs between loss and constraint violation: this is depicted for a simple example in Figure 1B.

Multiple equivalent optima may cause a non-monotonic relation between λ and the constraint satisfaction level, similarly to what discussed in the previous paragraph.

Additionally, it may happen that different constrained optima are associated to the same multiplier, and to no other multiplier. In Figure 1A, for example, the multiplier λ_j = 1 is associated to all optimal solutions of PC(θ) with θ ≤ θ^*; no other multiplier is associated to the same solutions. Unless some kind of tie breaking technique is employed, this situation makes specific constrained optima impossible to reach.

Inaccessible Constrained Optima We next proceed to investigate whether an optimum of the constrained formulation may be associated to no multiplier value: any such point would be completely unattainable via Algorithm 1. We have that:

**Theorem 2** An optimal solution w^* for PC is optimal for PR iff there exists a multiplier vector λ that satisfies:

\[
\max_{w \in W} R(w, \lambda) \leq \lambda_j\min_{w \in W} R(w, \lambda) \quad (12)
\]

with:

\[
R(w, \lambda) = -\frac{\Delta L(w, w^*) + \lambda_j \Delta C_j(w, w^*)}{\Delta C_j(w, w^*)} \quad (13)
\]

In the theorem, we refer with \(\Delta C(w, w^*)\) to the difference \(C(w) - C(w^*)\) and with \(\Delta L(w, w^*)\) to the difference \(L(w) - L(w^*)\). Moreover, \(\lambda_j\) refers to the set of all multiplier indices, except for \(j\). Intuitively, every assignment for which constraint \(j\) has a lower degree of violation than in \(w^*\) enforces an upper bound on \(\lambda_j\); every assignment for which the violation is higher enforces a lower bound.

**Proof 2** Let \(w^*\) be a PC optimum for some threshold θ; this implies that \(w^*\) is also optimal for a tightened threshold, i.e. for \(\theta = C(w^*)\). We therefore have:

\[
L(w) \geq L(w^*) \quad \forall w \in W, C(w) \leq C(w^*) \quad (14)
\]
An Analysis of Regularized Approaches for Constrained Machine Learning

We are interested in the conditions for \( w^* \) to be optimal for the regularized formulation, for some multiplier vector \( \lambda \). This is true iff:

\[
L(w) + \lambda^T C(w) \geq L(w^*) + \lambda^T C(w^*) \quad \forall w \in W
\]

which can rewritten as:

\[
\lambda^T \Delta C(w, w^*) + \Delta L(w, w^*) \geq 0 \quad \forall w \in W
\]

(15)

If \( \Delta C(w, w^*) = 0 \), then Equation (16) is trivially satisfied for every multiplier vector, due to Equation (14). Otherwise, at least some component in \( \Delta C(w, w^*) \) will be non-null, so that we can write:

\[
\lambda_j \Delta C_j(w, w^*) + \lambda^T \Delta C_j(w, w^*) + \Delta L(w, w^*) \geq 0
\]

(16)

If \( \Delta C_j(w, w^*) < 0 \), we get:

\[
\lambda_j \leq -\frac{\Delta L(w, w^*) + \lambda^T \Delta C_j(w, w^*)}{\Delta C_j(w, w^*)} \quad \forall w \in W \mid C_j(w) < C_j(w^*)
\]

(17)

I.e. a series of upper bounds for \( \lambda_j \). If \( \Delta C_j(w, w^*) > 0 \), we get:

\[
\lambda_j \geq -\frac{\Delta L(w, w^*) + \lambda^T \Delta C_j(w, w^*)}{\Delta C_j(w, w^*)} \quad \forall w \in W \mid C_j(w) > C_j(w^*)
\]

(18)

I.e. a series of lower bounds on \( \lambda_j \). From these the original result is obtained.

The main consequence of Theorem 2 is that the reported system of inequalities may actually admit no solution, meaning that some constrained optima may be unattainable via Algorithm 1. This is the case for the optimum \( w^* \) (for threshold \( \theta^* \)) in the simple example from Figure 2, since any multiplier value will result in an unbounded regularized problem. This is a potentially serious limitation of regularized methods: the actual severity of the issue will depend on the specific properties of the loss, regularizer, and ML model being considered.

Numerical Issues Theorem 2 highlights another potential issue of regularized approaches, arising when assignments with constraint violations arbitrarily close to \( C(w^*) \) exist. In such a situation, the denominator in Equation (13) becomes vanishingly small: depending on the properties of the loss function, this may result in arbitrarily high lower bounds or arbitrarily small upper bounds. Informally, reaching a specific optimum for the constrained problem may require extremely high or extremely low multipliers, which may cause numerical issues at training time. A simple example is depicted in Figure 2B, where a regularizer with vanishing gradient and a loss with non-vanishing gradient are combined. In such a situation, the constrained optimum \( w^* \) is reached via Algorithm 1 only for \( \lambda \rightarrow \infty \).

Differentiability Besides the ones reported here, one should be wary of pitfalls that are not immediately related to Algorithm 1. Many regularization based approaches for constraint injection, for example, require differentiability of the \( C \) function, which is often obtained by making approximations. For instance, in Equation (3) differentiability does not hold due to the use of binary variables; relaxing the integrally constraint address the issue, but allows to satisfy the constraints by assigning 0.5 to all outputs, i.e. by having completely uncertain, rather than balanced, predictions.

Figure 2: (A) Unattainable Constrained Optimum; (B) Numerical Issues for \( w^* \)
3 Conclusions

Combining the ML and optimization paradigms is a very interesting research avenue still under ongoing exploration by the AI community. Integrating learning and optimization will lead to approaches better suited for ethical and trustworthy AI (e.g. by making sub-symbolic models fair and explainable). A possible method to merge these paradigm consists in adding a regularization term to the loss of a learner, to constrain its behaviour. In this note, we offered a preliminary discussion on a particular aspect of this problem, namely we tackle the issue of finding the right balance between the loss (the accuracy of the learner) and the regularization term (the degree of constraint satisfaction); typically, this search is performed by adjusting a set of multipliers until the desired compromise is reached. The key results of this paper is the formal demonstration that this type of approach, albeit well suited for many practical circumstances, cannot guarantee to find all optimal solutions. In particular, in the non-convex case there might be optima for the constrained problem that do not correspond to any multiplier value. This result clearly hinders the applicability of regularizer-based methods, at least unless more research effort is devoted to discover new formulations or algorithms.

References

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