Abstract

This paper introduces a novel algorithm for a class of weakly supervised learning tasks. The considered tasks are posed as joint optimization problems in the continuous model parameters and the (a-priori unknown) discrete label variables. In contrast to prior approaches such as convex relaxations, we decompose the nonconvex problem into purely discrete and purely continuous subproblems in a way that is amenable to distributed optimization by the Alternating Direction Method of Multipliers (ADMM). This approach preserves integrality of the discrete label variables and, for a reparameterized variant of the algorithm using kernels, guarantees global convergence to a critical point. The resulting method implicitly alternates between a discrete and a continuous variable update, however, it is inherently different from a discrete-continuous coordinate descent scheme (hard EM). In diverse experiments we show that our method can learn a classifier from weak supervision that takes the form of hard and soft constraints on the labeling and outperforms hard EM in this task.

1 Introduction

One of the main challenges in machine learning is the exact annotation of training data, which has become a typical bottleneck of modern machine learning applications. For this reason, substantial research has been devoted to models and algorithms for weakly and semi-supervised learning that take advantage of weakly and sparsely labeled data.

Moreover, the (human guided) annotation process may become more efficient, in case the training algorithm can exploit structured a-priori knowledge about labels instead of more expensive exact annotation. Such knowledge may take the form of hard or soft constraints on feasible labelings, or, more generally, of a supervision function which we refer to as a weak supervisor.

In this paper we consider weakly supervised classification problems that, given a set of training instances $I := \{1, \ldots, N\}, N \in \mathbb{N}$, represented by their feature vectors $x_i \in \mathcal{X} \subset \mathbb{R}^d, d \in \mathbb{N}, i \in I$, can be modeled in terms of a joint minimization problem in (a-priori unknown) discrete label variables $Y$ and continuous model parameters $W$:

$$
\min_{W,Y} \frac{1}{N} \sum_{i=1}^{N} \ell(W, x_i, y_i) + R(W) + S(Y). \tag{1}
$$

The different terms in the objective correspond to:

(i) An empirical risk defined as the sum of loss terms $\ell(W, x_i, y_i)$ for individual training instances $i \in I$. Each loss term depends on the continuous model parameters $W$ and the discrete label variable...
$y_i \in \mathcal{Y}$ given in one-hot encoding, where $\mathcal{Y}$ denotes the finite set of one-hot encodings for $C$ distinct classes. Typical choices are, for instance, the Crammer and Singer multi-class SVM loss [8], or the softmax loss, in combination with a linear classifier, in which case $W \in \mathbb{R}^{d \times C}$. The loss may also be given as a structured or latent variable SVM loss [33, 40] or it may incorporate a nonlinear classifier such as a neural network. However, in this work we focus on convex loss functions, as the individual loss terms can typically be optimized efficiently via duality.

(ii) A regularizer $R(W)$ on the model parameters. Typical choices are, for instance, the $\ell_1$-norm or the squared Frobenius norm, that we denote by $\| \cdot \|_2^2$.

(iii) A weak supervisor function $S: \mathcal{Y}^N \rightarrow \mathbb{R} \cup \{ \infty \}$, that assigns a (possibly infinite) cost to any labeling $Y \in \mathcal{Y}^N$ of the $N$ instances. We define the feasible set of the supervisor as $\text{dom}(S) := \{ Y : S(Y) < \infty \}$.

Problem (1) admits diverse forms of weak supervision, by modeling the supervisor in different ways. For instance, the supervisor can be defined in terms of the objective of a tree-structured Markov Random Field (MRF):

$$S(Y) = \sum_{i \in I} u_i(y_i) + \sum_{ij \in E} p_{ij}(y_i, y_j),$$

where $u_i : \mathcal{Y} \rightarrow \mathbb{R} \cup \{ \infty \}$ and $p_{ij} : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R} \cup \{ \infty \}$ are the unary, respectively pairwise potentials, and $E \subset \binom{I}{2}$ defines an undirected forest on $I$. The tree structure guarantees efficiency of our method. With the unary potentials we may model for a certain instance $i$ the likelihood of it to belong to a particular class. We may also rule out specific class labels, which we refer to as negative labels. With the pairwise potentials we can model that certain label combinations assigned to pairs of instances are more likely than others. This enables the human annotation of similarities and dissimilarities of training instances without specifying any exact labels. For a supervisor with only pairwise terms and a quadratic distance loss, the model (1) specializes to constrained $k$-means clustering [34, 2].

Alternatively, from a discrete optimization perspective, we may interpret the resulting model as the attempt to learn (additional) unary potentials $u'_i : \mathcal{Y} \rightarrow \mathbb{R}$ of an MRF in a joint fashion: Let $(W^*, Y^*)$ be a minimizer of (1), then the $u'_i$ are given via the loss function $u'_i(y_i) = \ell(W^*, x_i, y_i)$. For instance in semantic segmentation, model (1) allows for learning a pixel-wise data term jointly with the segmentation using raw patch-features.

The supervisor can also be modeled in terms of a min cost flow objective [4] for an a-priori known flow network $G$ with a-priori unknown costs [3, 2]. In [2] this is used to efficiently model a constraint on the labeling $Y$, that balances the assignment of instances to different classes. More abstractly, we may interpret the resulting model as the attempt to learn an “optimal” cost matrix $\gamma$ for $G$ jointly with the flow. Here, the entries of the cost matrix have the form $\gamma_{ij} = \ell(W^*, x_i, y_i)$, where $(W^*, Y^*)$ is a minimizer of (1). This may have applications for instance in multi-object tracking, which is often modeled in terms of a min cost flow problem [42].

1.1 Related Work

A typical approach for tackling problems of the form (1) is via a coordinate descent scheme in the discrete and the continuous variables [3, 34, 2]. In the context of MAP-inference in latent variable models, this is referred to as hard Expectation-Maximization (EM). For instance, with a squared distance loss, and in the absence of any supervision, problem (1) specializes to $k$-means clustering. The latter is commonly tackled by Lloyd’s algorithm [22] that employs alternating optimization to compute a local minimum. Due to its simplicity and low complexity the method is still appealing and therefore recent research is devoted to improvements [19, 13, 56, 27]. A particular issue with Lloyd’s algorithm is, that its performance is highly sensitive to the initialization. The efficient computation of provably good seedings is therefore studied in [1].

The $k$-means clustering problem can be extended so as to account for combinatorial soft and hard constraints on the clustering such as the discussed pairwise constraints [34] or a balancing constraint [3, 2]. This is commonly referred to as constrained clustering [2].

For loss functions that are more common in classification, such as the hinge loss, the alternating optimization scheme breaks down, because it converges early to a poor local optimum [41]. Therefore, specialized algorithms based on SDP relaxations [38, 17] or CCCP [43] have been devised for a
generally unconstrained setting. An SDP relaxation approach for weakly supervised learning in the context of multinomial logistic regression is proposed by [17]. While convex SDP relaxation methods are robust regarding initialization, on the downside they generally do not scale well to larger problem instances: The approach by [17] has a per-iteration complexity of $O(N^3)$. Moreover, those methods typically need to eliminate or relax the discrete variables. This has two important drawbacks: (i) It is in general very difficult to strictly impose combinatorial constraints on the labeling and (ii) a post-processing (rounding) method is usually employed, which degrades the quality of the final solution compared to the optimal (relaxed) solution [17].

In order to overcome those issues, we present a different approach that is amenable to efficient optimization by the Alternating Direction Method of Multipliers (ADMM). ADMM, coined by [14, 12] is traditionally applied in convex optimization where it converges under mild conditions [11, 9]. More recently, it has been applied as a heuristic method to a variety of discrete and NP-hard problems as well [31, 25, 23, 16, 32]. In particular, the application of ADMM to quadratic mixed integer programs has recently been studied by [16, 32]. Typically, those approaches do not admit a convergence guarantee and the solution found by ADMM is generally not integral. Therefore, a rounding step may be integrated into the ADMM formulation [32]. However, as reported by the authors this may lead to an unstable algorithm.

Whereas ADMM converges under very general assumptions for the convex case, the convergence in a more restrictive nonconvex setting has recently been proven [15, 21, 35]. In this case, however, the required assumptions are fairly strong.

1.2 Contribution

This paper makes two contributions.

Firstly, we propose a decomposition of the generally NP-hard weakly supervised learning problem (1) into purely discrete and purely continuous sub-problems. The discrete-continuous splitting we propose has three advantages: (a) it is amenable to optimization by ADMM, (b) it guarantees global convergence to a critical point of the objective function for classifiers parameterized by a kernel, and (c) it maintains integrality of the discrete labels (without postprocessing or rounding).

Secondly, we solve challenging instances of Problem (1) experimentally, by means of ADMM, demonstrating the following advantages over alternative methods:

Compared to alternating optimization by hard EM, which have been shown in [41] to be prone to bad local minima for classification loss functions, our algorithm is robust to initialization and systematically produces good local optima.

Compared to the SDP relaxation proposed in [17] whose optimization has worst-case $O(N^3)$ for a kernelized classifier, our algorithm has worst-case time complexity $O(N^2)$ for a classifier parameterized by a kernel. In addition, it allows for more general forms of weak supervision and, on the task of semi-supervised learning produces more consistent results.

2 Discrete-Continuous Splitting

The remainder of this section is organized as follows: In Section 2.1 we describe the consensus ADMM framework employed for a discrete-continuous decomposition of problem (1), and interpret our step size update as a form of graduated nonconvexity. In Section 2.2 we discuss a novel discrete-continuous proximal mapping, that preserves integrality of the discrete variable and therefore is considered the central part of our method. In Section 2.3 we further describe a kernelized variant of our formulation that admits a convergence guarantee and scales, for a separable supervisor, as the supervised training of a kernel SVM.

2.1 Discrete-Continuous Consensus ADMM

Finding good feasible solutions of an NP-hard problem via an ADMM approach has become popular in recent years [31, 25, 23, 16]. Most of the time the idea is to write an objective function $F$ as a sum

3
of $N$ objective functions $F_i$ that are easy to optimize. As a consequence, one is interested in

$$\min_{Y_i, Y_i, i=1}^{N} \sum_{i=1}^{N} F_i(Y_i)$$

subject to $Y_i = Y, \forall i$. \(3\)

The idea of ADMM is to relax the couplings $Y_i = Y$ and successively strengthen these constraints in each iteration so that the “independent” solutions $Y_i$ converge towards a consensus solution $Y$. Nonetheless, this approach does not always provide discrete solutions. Therefore, a post-processing method is usually employed and the final (rounded) solution need not be close to the optimal (relaxed) solution.

Problem \(1\) is NP-hard in general as well, as it subsumes $k$-means clustering. We propose to reformulate the problem in a way that preserves integrality of the discrete variables.

Proposed Decomposition. In contrast to the discrete decomposition of \(3\) with respect to $Y$, we propose a decomposition with respect to the continuous variables $W$: We introduce continuous auxiliary variables $W_i$ and linear consensus constraints $W_i = W$ on a per-instance level, which (in case the constraints are absent) for fixed $Y$ decouples the loss terms in $W$. This leads to the following equivalent constrained reformulation of problem \(1\):

$$\min_{Y, W, \{W_i\}_{i=1}^{N}} \frac{1}{N} \sum_{i=1}^{N} \ell(W_i, x_i, y_i) + R(W_i) + S(Y)$$

subject to $W_i = W, \forall i$. \(4\)

Clearly, this formulation is different from the consensus setting in \(3\) for discrete NP-hard optimization, due to the presence of the discrete variables $Y$ and the supervisor $S(Y)$. Moreover, the discrete variable $Y$ is another “complicating variable”, that also couples all summands via the supervisor.

In order to fit our formulation into the general consensus model \(3\) auxiliary variables also for the $y_i$ have to be introduced. As explained above, with this approach integrality of $Y$ cannot be guaranteed. Therefore, we pursue a different and more efficient strategy: Instead of further decomposing the problem into even smaller subproblems, we do not let ADMM operate on the discrete variables and instead encapsulate the minimization over $Y$ within a function $L$:

$$L(W_1, \ldots, W_N) := \min_Y \frac{1}{N} \sum_{i=1}^{N} \ell(W_i, x_i, y_i) + R(W_i) + S(Y).$$ \(5\)

As an important consequence the function $L$ has to be optimized efficiently within the algorithm. This becomes the central part of our method and therefore we devote Section \(2.2\) to this problem. Further, we note that in case the supervisor is the trivial zero function, our approach specializes to a decomposition that is typically used in supervised learning with ADMM \([10, 5]\).

Using \(5\), problem \(4\) can be compactly written as

$$\min_{W, \{W_i\}_{i=1}^{N}} L(W_1, \ldots, W_N)$$

subject to $W_i = W, \forall i$. \(6\)

For a particular penalty parameter $\rho$, the ADMM iterates for the above problem are given as

$$\{W_i^{t+1}\}_{i=1}^{N} = \arg \min_{\{W_i\}_{i=1}^{N}} L(W_1, \ldots, W_N) + \frac{\rho}{2} \sum_{i=1}^{N} \|W_i - W_i^t + \lambda_i^t\|^2$$

$$W_i^{t+1} = \frac{1}{N} \sum_{i=1}^{N} \rho W_i^{t+1} - \lambda_i^t$$

$$\lambda_i^{t+1} = \lambda_i^t + \rho(W_i^{t+1} - W_i^{t+1}) \forall i.$$ \(7\)
Graduated Nonconvexity via Penalty Parameter Update. Next we focus on the choice of the penalty parameter $\rho$, as a carefully chosen parameter may drastically improve the quality of the solutions found by ADMM in nonconvex optimization [39]. In our method we choose $\rho$ adaptively: More precisely, we increase $\rho$ slowly during the iterations, starting from a small value in the order of $10^{-4}$. This, in practice, leads to much better local optima in terms of objective value and makes the algorithm robust towards initialization. In this section we provide an interpretation of this behavior in the context of graduated nonconvexity:

In [24] the authors observe that consensus ADMM approaches a projected subgradient descent on the convex, negative Lagrangian dual function, referred to as dual decomposition (DD) [19], if the penalty parameter $\rho$ is close to zero. This carries over also to our algorithm. Whereas in [24] a convex objective is optimized, and therefore the problems solved by DD and ADMM are equivalent, in our case DD solves a convex relaxation that we characterize in the following Observation:

**Observation 1.** Let the supervisor $S$ be separable, i.e. $S(Y) = \sum_i S_i(y_i)$. Then the Lagrangian dual problem of (4) is equivalent to the following convex relaxation

$$\min_W N \sum_{i=1}^N \tilde{\ell}(\cdot, x_i)^*(W)$$

where $\tilde{\ell}(W, x_i) = \frac{1}{N} \min_{y_i \in Y} \ell(W, x_i, y_i) + S_i(y_i) + R(W)$ and $\tilde{\ell}(\cdot, x_i)^*$ denotes the convex biconjugate of $\tilde{\ell}(\cdot, x_i)$, i.e. the largest lower semi-continuous convex underapproximation of $\tilde{\ell}(\cdot, x_i)$.

The above result can be obtained via a simple computation, starting from the definition of the Lagrangian dual problem using the definition of the Fenchel-Legendre convex conjugate and Fenchel duality. We provide a formal proof in the Appendix A.1.

We observe that, in the absence of the supervision function and the regularizer, for typical loss functions such as the hinge loss or the logistic loss this convex relaxation yields the trivial zero function. However, if weak supervision and a regularizer is present, the convex relaxation becomes meaningful. Clearly, if $\ell$ and $R$ are convex and the supervisor is very certain about one particular labeling, the problem approaches a convex one. In that sense the convex relaxation becomes tighter as the supervisor is less uncertain about the labeling.

In the light of this observation, we may informally interpret a nondecreasing update schedule for $\rho$ as a form of graduated nonconvexity [37]. Continuation methods for graduated nonconvexity have for instance been applied for the optimization of semi-supervised versions of the SVM [6].

Local Convergence. Global convergence of Algorithm 1 can so far not be guaranteed by existing theory, since $L$ is nonsmooth [35]. Clearly, $L$ is continuous and piecewise convex with finitely many convex pieces, as it is given as a minimum over finitely many continuous convex functions. Therefore, there are only finitely many points, at which convex pieces join up so that they form a strict local maximum. This means that for any local minimum of the objective there exists a sufficiently small neighborhood on which the objective is convex. Local convergence of DC-ADMM, may therefore be deduced from existing convergence results for convex objectives [5].

In practice, we observe that the algorithm converges also globally, once the penalty parameter $\rho$ is large enough. A mathematical proof is an interesting open problem and subject to future research.

2.2 Discrete-Continuous Proximal Mapping

In order to state the final Algorithm 1 which we refer to as discrete-continuous ADMM (DC-ADMM), it remains to discuss the solution of the subproblem: In this section we devise an efficient Algorithm 2 that computes the $W_i$ update in (7) and, as a byproduct, outputs the corresponding optimal labeling $Y$.

This update may be interpreted as a proximal step on the nonconvex, nonsmooth function $L$, which is defined as the minimum over in general exponentially many functions. For some step size $\sigma > 0$ the proximal mapping $P_{\sigma F}$ and the corresponding the Moreau envelope $M_{\sigma F}$ of a proper, lower
We note, that $\in S$ To this end we assume that the minimization of both the discrete function $\text{arg min}_W \ell(W, x_i, y_i) + R(W_i) + \frac{\rho}{2} \| W_i - W^t \|^2 + \lambda_i' \rho^2$.

The proximal mapping that we like to solve for the $W$ objective is separable w.r.t. $W$. For the general case of a nonseparable supervisor $S$ we may proceed similarly, as for fixed $Y$ the objective is separable w.r.t. $W_i$. The difference is, that the optimal labeling $Y^*$ needs to be computed,
before the optimal values are looked up. The optimal labeling $Y^*$ is given via the solution of

$$Y^* = \min_Y \langle \gamma, Y \rangle + S(Y),$$

(12)

which can for instance be obtained via belief propagation for the special case (2) or the solution of a min cost flow problem or, in a more general setting via integer linear programming. Here, the matrix $\gamma$ specifies an additional linear cost on $Y$, which corresponds to an additional unary potential for the special case (2).

It may be interpreted as a message, that guides the supervisor to adapt the labeling towards a more “optimal” classifier. The latter is determined via a tradeoff between the distance to the current consensus variable $W^t - \lambda^t/\rho$ and low loss value.

The optimal values $W^*_i$ can be read off from the solution of (11) via

$$W^*_i = \sum_{j=1}^C y^*_i j B_{ij}.$$  

We summarize this procedure in Algorithm 2.

**Distributed Optimization.** Overall, the $W_i$ update requires the solution of only $N \cdot C$ instead of to $N^C$ many independent and small-scale continuous minimization problems and one additional discrete problem. As a positive side effect, this allows for the distributed solution of the subproblems for example on a GPU. Subsequently, the solution of the discrete problem and the update of the consensus variable is carried out by the “master” after gathering the solutions of the subproblems. Distributed optimization is considered one of the main advantages of ADMM in supervised learning [10, 5].

**Exploit Duality.** In case $\ell(\cdot, x_i, y_i)$ is convex and lower semicontinuous in the first argument, the independent subproblems (11) may be solved efficiently via duality: For the employed loss functions the dual problem scales linearly with the number of training samples (which is equal to one in our case), whereas the primal scales linearly with the feature dimension $d$ which may be high. For the Crammer and Singer multiclass SVM loss [8] for instance, there exists an efficient variable fixing algorithm [18] for solving the dual. Via the Lambert-$W$ function the dual problem for the softmax loss can be reduced to a one-dimensional nonlinear equation [20], that may be solved by Newton’s or Halley’s method. For simpler special cases such as the hinge loss, there exists a closed form solution.

2.3 A Tractable and Convergent Kernel-Formulation

Finally, for a kernel setting, we consider a different ADMM formulation that we find more appealing than DC-ADMM in two ways: Firstly, for separable supervisors, the per-iteration complexity is $O(N^2)$ so that our method scales as fully supervised training of a kernel SVM. Secondly, it admits a convergence guarantee (under mild assumptions) by existing theory. We note that convergence of ADMM in nonconvex optimization cannot be taken for granted in general as it is a tool traditionally used in convex optimization.

**Reparameterization for a Kernel Setting.** For the kernel setting we assume that the loss $\ell(\cdot, y_i)$ is given as a function of classifier scores $\phi(x_i)^T W$, where $\phi$ denotes a possibly infinite dimensional feature map, and the regularizer is given as $R(W) = \nu \|W\|_2^2$, with $\nu > 0$. Then, for a fixed labeling $Y$, the representer theorem [29] states that the parameters $W = \Phi(X)\alpha$ can be substituted via their representation $\alpha$ in terms of the matrix features $\Phi(X)$. We use this to employ a change of representation, in our objective function. Let $K$ denote the kernel matrix associated to $\Phi(X)$. Using the same trick as in Section 2.1 we may encapsulate the minimization over $Y$ within a function $L$ so that ADMM formally operates on the continuous variables only: Let $L$ be given as

$$L(\beta) = \min_Y \frac{1}{N} \sum_{i=1}^N \ell(\beta_i, y_i) + S(Y).$$

(13)

Then, we may reformulate problem (1) (in a constrained form) as

$$\min_{\alpha, \beta} L(\beta) + \nu(\alpha, K\alpha)$$

subject to $K\alpha = \beta$. 

(14)
The iterates of ADMM are by definition given via

$$\beta^{t+1} = \arg \min_{\beta} L(\beta) + \frac{\rho}{2} \|\beta - K\alpha^t + \lambda^t/\rho\|^2$$

$$\alpha^{t+1} = \arg \min_{\alpha} \nu\langle \alpha, K\alpha \rangle + \frac{\rho}{2} \|K\alpha - \beta^t + 1 - \lambda^t/\rho\|^2$$

$$\lambda^{t+1} = \lambda^t + \rho(\beta^t - K\alpha^t).$$

Again, the update of the variable $\beta$, given via a proximal mapping can be performed using an algorithm similar to Algorithm 2. The update of the variable $\alpha$, can be obtained via the solution of a normal equation using either a cached eigenvalue decomposition of the kernel matrix, or an iterative algorithm such as conjugate gradient. We observe that in practice only a small number of conjugate gradient iterations are necessary. Empirically, the number of required (outer) ADMM-iterations rather depends on the desired accuracy, the update schedule for the penalty parameter and the complexity of the model, than on the number of training examples. This observation is supported by the fact, that in convex optimization, ADMM may converge slowly to a high accuracy result (sublinear convergence). However, in practice, ADMM usually converges to modest accuracy—sufficient in machine learning tasks—with a few dozen iterations [5]. In this sense the method asymptotically scales as fully supervised training of a kernel SVM for separable supervisors.

The following proposition states that the explicit ADMM-scheme (15) for our problem produces a sequence that converges to a critical point of the objective function.

**Proposition 1.** Let the kernel matrix $K$ be positive definite and let $f$ be either globally Lipschitz in $\beta$, or locally Lipschitz and lower bounded and let $\nu > 0$. Then there exists a penalty parameter $\rho$, large enough, so that the sequence produced by the ADMM scheme applied to (14), converges to a stationary point of the augmented Lagrangian of (14).

The proof can be obtained by verifying that the assumptions in [35] are met. A formal proof is provided in the Appendix A.2.

**Discussion of the Assumptions.** We note that most of the considered loss functions are Lipschitz continuous including the hinge loss and the logistic loss.

Further, note that in general the kernel matrix $K$ is not positive definite but positive semidefinite. However, for the strictly positive definite radial basis function (RBF) kernel, $K$ is positive definite. Although the matrix is ill-conditioned and its smallest eigenvalues may be numerically around zero this does not harm in practice: Due to the presence of the regularizer, the solution of the least squares problem for the $\alpha$-update becomes unique.

In order to enforce theoretical convergence also for general kernels, one may add a small constant to the diagonal of the kernel matrix $K := K + cI$ without fundamentally changing the model. Further, for the hinge loss this is can be interpreted as a transition from an $\ell_1$-norm soft margin to an $\ell_2$-norm soft margin in the context of the SVM-model.

In all conducted experiments we have observed, that ADMM is stable and globally converges to a (verifiable) critical point of the objective, even if the kernel matrix is not strictly positive definite.

### 3 Experiments

In this section, we provide illustrative experiments to demonstrate that our method is able to learn a model in diverse weakly supervised scenarios.

**3.1 Proof of Concept**

As a proof of concept we conduct two small toy experiments with synthetic data sampled from 2D moon-shape distributions (600 samples, 150 per class). Instead of providing exact labels for training, we provide synthetic complex combinatorial supervision that is much weaker in the sense that it is highly ambiguous and yet involves complicated constraints.
Learning from Negative Labels and Pairwise Constraints. In the first experiment we attach to each training example \( i \) a randomly chosen negative label \( \bar{y}_i \neq y^*_i \) (where \( y^*_i \) is the true label of the training example) that only indicates that the training example \( i \) does not belong to class \( \bar{y}_i \). Additionally, we provide the algorithm with randomly sampled tree-structured pairwise should-link and should-not-link constraints, which indicate that certain pairs of training examples \( (i, j) \) should belong to the same class \( (y_i = y_j) \) or to distinct classes \( (y_i \neq y_j) \). Again, the pairwise constraints are in accordance with the true training labels. Mathematically, the supervisor is given in terms of a tree-structured MRF-objective (2), where the unary resp. pairwise potentials are given as

\[
\begin{align*}
    u_i(y_i) &= \begin{cases} 
        \infty & \text{if } y_i = \bar{y}_i \\
        0 & \text{otherwise,}
    \end{cases} \\
    p_{ij}(y_i, y_j) &= \begin{cases} 
        0 & \text{if } y_i = y_j \text{ (respectively } y_i \neq y_j) \\
        T & \text{otherwise,}
    \end{cases}
\end{align*}
\]

for a fixed penalty \( T > 0 \). This form of supervision is depicted in Figure 1a. The negative labels are visually interpreted as follows: The colored marker that is not present within some moon, but all the other moons, represents the true class of this cluster (cf. Figure 1a). It can be seen that our method determines a reasonable classifier and a corresponding labeling that is in accordance with the supervisor. The resulting training error of our method is 1.3%.

![Figure 1](image_url)

(a) Negative labels and pairwise constraints. The negative labels are indicated via the colored markers and the should-(not)-link constraints are visualized by solid (dashed) edges. (b) Solution of the (ambiguous) combinatorial problem only. Here, markers correspond to the determined class labels. (c) Solution found by supervised SVM training with 1-vs-all decision boundaries. (d) Solution found by our method with 1-vs-all decision boundaries. The resulting training error of our method is 1.3%.

Learning from Balancing Constraints. In this experiment we sample 25 (possibly overlapping) mini batches \( B_k \subset \mathcal{I} \) of cardinality 25 from the training set. The synthetic supervision in this experiment is given in terms of a set of balancing constraints on the batches. More precisely, it restricts the maximal deviation of the determined labeling \( Y \) from the true labeling to a given bound within each batch \( B_k \). Mathematically, the supervisor \( S \) is given as

\[
S(Y) = \begin{cases} 
    0 & \text{if } L^k_j \leq |\{i \in B_k : Y_{ij} = 1\}| \leq U^k_j \text{ for all } 1 \leq j \leq C \text{ and } 1 \leq k \leq 25 \\
    \infty & \text{otherwise.}
\end{cases}
\]

where the bounds \( L^k_j \) and \( U^k_j \) are chosen such that the number of samples assigned to class \( j \) deviates by at most 3 from the true number within batch \( B_k \).

We optimize the arising linear program (12) with the dual-simplex method and observe that the solution is integral in our experiments. This ensures optimality.

We compare our method to constrained kernel k-means and hard EM on this task (see Figure 2). Similarly to [4, 34, 2], we apply k-means in the RBF-kernel space [30] and solve the E-step w.r.t. to (17). As a second baseline we solve the proposed model (1) with a discrete-continuous coordinate descent, which we refer to as hard EM. For both, hard EM and our method we choose an SVM-model. It can be seen that both hard EM (Figure 2a) and constrained kernel k-means (Figure 2b) get stuck in a poor local minimum, that is mainly guided by the initial solution of the combinatorial supervision problem (initial E-step) depicted in Figure 2a. As it can be seen in Figure 2a, solving the combinatorial problem only does not suffice to determine the true labels. Even worse, it gives the wrong cues for the true clusters.

As the performance of hard EM is highly sensitive to initialization, it may be improved by providing the algorithm with an initialization, that is more consistent with the actual clusters and not only with the weak supervision. However, finding good initializations w.r.t. complex combinatorial supervision
may in general become as difficult as solving the original problem. For that reason, we can initialize hard EM only with random classifiers resp. cluster centers in our experiments.

Since our proposed method is robust regarding the initialization, we observe that it overcomes the chicken-and-egg problem of finding good initializations w.r.t. weak supervision. It can be seen in Figure 2d that our method is able to infer the true labels of most training instances and finds a reasonable classifier, even though initially the wrong cues are given by the supervisor and all variables are initialized with zero. The obtained training errors are 66.6% for constrained RBF-kernel \( k \)-means, 68.5% for hard EM and 2.5% for our method.

3.2 Handwritten Digits Classification with Weak Supervision.

As another experiment we train a weakly supervised RBF-kernel SVM on the popular MNIST handwritten digits data set. We restrict ourselves to a balanced subset of 10000 images from the original training set (which consists of 60000 images from 10 different classes). Instead of using the true class labels from the training set, we randomly attach \( k \in \{1, \ldots, 8\} \) many negative labels to each training example, which only indicate classes that the training example does not belong to.

In a second setup we additionally provide the algorithm with randomly sampled pairwise must-link and must-not-link constraints that are in accordance with the ground truth. As a baseline we use the same SVM-model trained in a fully supervised fashion, which achieves a test error of 3.37%.

Figure 3 reports the increase of incorrectly predicted training labels and test error compared to the baseline model depending on the number of negative labels \( k \). It can be seen that the absolute test error increases by up to roughly 4% for only 1 negative label and by 2% in case additional pairwise constraints are present. This suggests that it is possible to learn a reasonable classifier without using any true class labels.

3.3 Comparison with SDP Relaxation.

Finally, we compare to an SDP relaxation method for weakly supervised multinomial logistic regression by [17] on the task of semi-supervised learning. We consider the standard SSL benchmark [7] for a comparison also used by [17]. The benchmark is a collection of several datasets, with varying feature dimensions and number of classes. Each dataset is provided with 12 splits into \( l = 10 \) or \( l = 100 \) labeled and \( N - l \) unlabeled samples. Whereas [17] incorporates an entropy prior on the labeling which favors an equal balance distribution, we adapt the supervisor \( S \) in a way that it restricts the solution to deviate at most \( b = 3 \) resp. \( b = 20 \) percent from the equal balance distribution. We use a MATLAB implementation, that is provided by the authors. For these experiments, we use the softmax loss and set the regularization parameter \( \nu = 0.0025 \), which corresponds to \( \lambda = 0.01 \) in the model by [17]. All values are averaged over 12 different splits. It can be seen in Table 1 that our method mostly performs better in terms of higher training accuracy. For \( l = 10 \) our method consistently produces better accuracies. Moreover, it produces more consistent results over the splits in terms of lower variances, which suggests that our method is more robust towards noise and poorly labeled data.

Figure 2: Comparison of constrained RBF-kernel \( k \)-means, hard EM (with RBF-kernel SVM-model), and the proposed method (with RBF-kernel SVM-model) on the task of learning from balancing constraints (17). 2a: Solution after initial E-step in hard EM. 2b: Solution found with constrained RBF-kernel \( k \)-means. 2c: Solution found with hard EM for an SVM-model. 2d: Solution found with our method for the same SVM-model. The obtained training errors are 66.6% for constrained RBF-kernel \( k \)-means, 68.5% for hard EM and 2.5% for our method.
Figure 3: Training an SVM classifier on MNIST with weak negative labels only (a) resp. weak negative labels and additional weak pairwise must-link and must-not-link constraints (b). We plot the absolute error increase in percent compared to a fully supervised model in relation to the number of negative labels per training instance. It can be seen that the absolute test error increases by up to roughly 4% and by 2% in case additional pairwise constraints are present.

Table 1: Comparison with the method of [17] on the SSL benchmark [7]. Reported are the average label accuracy (in %) and variance over the splits. It can be seen that our method mostly finds solutions with better accuracy and the accuracies are more consistent over the splits in terms of lower variance.

<table>
<thead>
<tr>
<th>Dataset</th>
<th>Linear Kernel</th>
<th>RBF Kernel</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>SDP</td>
<td>Ours (3%)</td>
</tr>
<tr>
<td>Digit1,10l</td>
<td>69.27±27.56</td>
<td>82.19±4.65</td>
</tr>
<tr>
<td>USPS,10l</td>
<td>57.72±13.73</td>
<td>64.58±3.37</td>
</tr>
<tr>
<td>BCI,10l</td>
<td>50.44±3.16</td>
<td>51.21±3.17</td>
</tr>
<tr>
<td>g241c,10l</td>
<td>49.88±38.92</td>
<td>55.42±3.95</td>
</tr>
<tr>
<td>g241n,10l</td>
<td>52.77±34.37</td>
<td>57.61±4.44</td>
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<tr>
<td>Digit1,100l</td>
<td>75.74±29.73</td>
<td>85.01±1.62</td>
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<tr>
<td>USPS,100l</td>
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<td>72.14±0.84</td>
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<tr>
<td>g241c,100l</td>
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<tr>
<td>g241n,100l</td>
<td>54.14±17.13</td>
<td>54.11±0.64</td>
</tr>
</tbody>
</table>

4 Conclusion

In this work we have presented a novel algorithm for mixed-integer problems in the context of weakly supervised learning. We devise a discrete-continuous decomposition that is amenable to optimization by ADMM. Like hard EM, this decouples the discrete and the continuous optimization which allows for solving complex discrete-continuous models. Yet, the approach is inherently different from a discrete-continuous coordinate descent scheme in the following sense: The discrete-continuous alternation is performed within a proximal mapping of a nonsmooth nonconvex function, and thus the discrete variable is hidden to ADMM. In diverse experiments we have demonstrated that our method can overcome the chicken-and-egg problem of finding good initializations w.r.t. combinatorial supervision (which hard EM relies on). This allows for learning a classifier from weak and abstract combinatorial supervision. Overall, we are optimistic that our method can open a door to more challenging mixed-integer optimization problems for weakly and semi-supervised learning.
A Proofs

A.1 Proof of Observation 1

Proof. Let the supervisor $S$ be separable, i.e. $S(Y) = \sum_i S_i(y_i)$ and let $\{\lambda_i\}_{i=1}^N$ be the Lagrange multipliers corresponding to the linear coupling constraints. Let $\bar{\ell}(\cdot, x_i)^*$ denote the Fenchel-Legendre convex conjugate of $\bar{\ell}(\cdot, x_i)$. Then the Lagrangian dual problem of (4) is given as

$$\max_{\{\lambda_i\}_{i=1}^N} \min_{W, \{W_i\}_{i=1}^N} N \sum_{i=1}^N \bar{\ell}(\cdot, x_i)(W) + \langle \lambda_i, W - W_i \rangle$$

Clearly, strong duality holds so that we may exchange the order of minimum and maximum and as the objective is separable w.r.t. the $\lambda_i$ further rewrite

$$\min_{W} \sum_{i=1}^N \max \langle \lambda_i, W \rangle - \bar{\ell}(\cdot, x_i)^*(\lambda_i),$$

which is by definition equal to the convex biconjugate of $\bar{\ell}(\cdot, x_i)$, i.e. the largest lower semi-continuous convex underapproximation of $\bar{\ell}$. \hfill \Box

A.2 Proof of Proposition 1

Proof. For the proof we consider the vectorized formulation of problem (14) meaning that $\alpha, \beta \in \mathbb{R}^{NC}$ and the linear constraints are given as $K\alpha - I\beta = 0$ where $K$ is redefined as $K = I \otimes K$. Since $K$ is positive definite, $K$ has full rank implying $\text{im}(K) = \mathbb{R}^{NC}$. Clearly, the objective in (14) is coercive over the feasible set $\{(\alpha, \beta) : K\alpha = \beta\}$ as $K$ is positive definite, $\nu > 0$ and the loss terms $\ell(\cdot, y_i)$ are either locally Lipschitz and lower bounded or globally Lipschitz. W.l.o.g. we may assume that $\ell(\cdot, y_i)$ is globally Lipschitz (cf. [35]). Then, also $\sum_{i=1}^N \ell(\beta_i, y_i)$ Lipschitz in $\beta$, as it is separable. Since $\text{dom}(S) = \{Y \in \mathbb{R}^N \mid S(Y) < \infty\}$ is finite, $L$ is the pointwise minimum over finitely many Lipschitz continuous functions and thus Lipschitz. Clearly, $\nu(\cdot, K\cdot)$ is Lipschitz differentiable. As $K$ is invertible, assumption A3 in [35] holds trivially. The global convergence to a stationary point of the augmented Lagrangian of (14) is a direct consequence of Theorem 1 in [35]. \hfill \Box
References


[37] Z. Wu. The effective energy transformation scheme as a special continuation approach to global optimization with application to molecular conformation. SIAM Journal on Optimization, 6(3):748–768, 1996.


