Faster Rates for Training Max-Margin Markov Networks

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Abstract

Structured output prediction is an important machine learning problem both in theory and practice, and the max-margin Markov network (M³N) is an effective approach. All state-of-the-art algorithms for optimizing M³N objectives take at least $O(1/\epsilon)$ number of iterations to find an $\epsilon$ accurate solution. Recent results in structured optimization suggest that faster rates are possible by exploiting the structure of the objective function. Towards this end [15] proposed an excessive gap reduction technique based on Euclidean projections which converges in $O(1/\sqrt{\epsilon})$ iterations on strongly convex functions. Unfortunately when applied to M³Ns, this approach does not admit graphical model factorization which, as in many existing algorithms, is crucial for keeping the cost per iteration tractable. In this paper, we present a new excessive gap reduction technique based on Bregman projections which admits graphical model factorization naturally, and converges in $O(1/\sqrt{\epsilon})$ iterations. Compared with existing algorithms, the convergence rate of our method has better dependence on $\epsilon$ and other parameters of the problem, and can be easily kernelized.

1 Introduction

In the supervised learning setting, one is given a training set of labeled data points and the aim is to learn a function which predicts labels on unseen data points. Sometimes the label space has a rich internal structure which characterizes the combinatorial or recursive inter-dependencies of the application domain. It is widely believed that capturing these dependencies is critical for effectively learning with structured output. Examples of such problems include sequence labeling, context free grammar parsing, and word alignment. However, parameter estimation is generally hard even for simple linear models, because the size of the label space is potentially exponentially large (see e.g. [3]). Therefore it is crucial to exploit the underlying conditional independence assumptions for the sake of computational tractability. This is often done by defining a graphical model on the output space, and exploiting the underlying graphical model factorization to perform computations.

Research in structured prediction can broadly be categorized into two tracks: Using a maximum a posteriori estimate from the exponential family results in conditional random fields (CRFs, [10]), and a maximum margin approach leads to max-margin Markov networks (M³Ns, [18]). Unsurprisingly, these two approaches share many commonalities: First, they both minimize a regularized risk with a square norm regularizer. Second, they assume that there is a joint feature map $\phi$ which maps $(x, y)$ to a feature vector in $\mathbb{R}^p$. Third, they assume a label loss $\ell(y, y'; x')$ which quantifies the loss of predicting label $y$ when the correct label of input $x'$ is $y'$. Finally, they assume that the space of labels $Y$ is endowed with a graphical model structure and that $\phi(x, y)$ and $\ell(y, y'; x')$ factorize according to the cliques of this graphical model. The main difference is in the loss function employed. CRFs minimize the $L_2$-regularized logistic loss:

$$J(w) = \frac{\lambda}{2} \|w\|^2 + \frac{1}{n} \sum_{i=1}^n \log \sum_{y \in Y} \exp \left( \ell(y, y'; x') - \langle w, \phi(x', y') - \phi(x', y) \rangle \right),$$

while the M³Ns minimize the $L_2$-regularized hinge loss

$$J(w) = \frac{\lambda}{2} \|w\|^2 + \frac{1}{n} \max_{y \in Y} \left\{ \ell(y, y'; x') - \langle w, \phi(x', y') - \phi(x', y) \rangle \right\}.$$  

\footnote{We discuss kernels and associated feature maps into a Reproducing Kernel Hilbert Space (RKHS) in the appendix.}
Figure 1: Illustration of stopping criterion monitored by various algorithms; convergence rates are stated with respect to these stopping criterion. $D(\alpha)$ is the Lagrange dual of $J(w)$, and $\min_w J(w) = \max_\alpha D(\alpha)$. Neither the primal gap nor the dual gap is actually measurable in practice since $\min_w J(w)$ (and $\max_\alpha D(\alpha)$) is unknown. BMRM (right) therefore uses a measurable upper bound of the primal gap. SVM-Struct monitors constraint violation, which can be also be translated to an upper bound on the primal gap.

| Optimization algorithm | Primal/Dual | Type of gap | Oracle for $M^iN$ | Convergence rate $O(\frac{1}{\lambda \log \frac{1}{\epsilon}})$ |
|------------------------|------------|-------------|-------------------|---------------------------------------------------|
| BMRM [22]              | primal     | $\geq$ primal gap | max               | $O\left(\frac{\lambda^2}{\lambda \epsilon}\right)$ |
| SVM-Struct [23]        | primal-dual| constraint violation | max               | $O\left(\frac{\lambda^2}{\lambda \epsilon}\right)$ |
| Extragradient [20]     | primal-dual| duality gap   | exp               | $O\left(\frac{\log \lambda}{\epsilon}\right)$ |
| Exponentiated gradient [2] | dual      | dual gap     | exp               | $O\left(\frac{\log \lambda}{\epsilon}\right)$ |
| SMO [17] Chapter 6     | dual       | dual gap     | max               | $\geq O\left(\frac{n^{1/3}}{\lambda \epsilon}\right)$ |
| Our algorithm          | primal-dual| duality gap  | exp               | $O\left(\frac{\log \lambda}{\epsilon}\right)$ |

Table 1: Comparison of specialized optimization algorithms for training structured prediction models. Primal-dual methods maintain estimation sequences in both primal and dual spaces. Details of the oracle will be discussed in Section 5. The convergence rate highlights the dependence on both $\epsilon$ and some “constants” that are often hidden in the $O$ notation: $n$, $\lambda$, and the size of the label space $|Y|$. No formal convergence rate is known for SMO on $M^iN$, therefore we quote the best known rate for training binary SVMs due to [12]. The term $G$ in the convergence rate of BMRM and SVM-Struct denotes the maximum $L_2$ norm of the features vectors $\phi(x, y)$. The convergence rate of Extragradient depends on $\lambda$ in an indirectly way.

A large body of literature exists on efficient algorithms for minimizing the above objective functions. A summary of existing methods, and their convergence rates (iterations needed to find an $\epsilon$ accurate solution) can be found in Table 1. The $\epsilon$ accuracy of a solution can be measured in many different ways. As Figure 1 depicts, different algorithms employ different but somewhat related stopping criterion. This must be borne in mind when interpreting the convergence rates in Table 1.

Since [1] is a smooth convex objective, classical methods such as L-BFGS can directly be applied [16]. Specialized solvers also exist. For instance a primal algorithm based on bundle methods was proposed by [22], while a dual algorithm for the same problem was proposed by [7]. Both algorithms converge at $O\left(\frac{1}{\lambda \log 1/\epsilon}\right)$ rates to an $\epsilon$ accurate solution, and, remarkably, their convergence rates are independent of $n$ the number of data points, and $|Y|$ the size of the label space. It is widely believed in optimization (see e.g. Section 9.3 of [6]) that unconstrained smooth strongly convex objective functions can be minimized in $O(\log 1/\epsilon)$ iterations, and these specialized optimizers also achieve this rate.

On the other hand, since [2] is a non-smooth convex function, efficient algorithms are harder to come by. SVM-Struct was one of the first specialized algorithms to tackle this problem, and [23] derived an
$O(G^2/\lambda \epsilon^2)$ rate of convergence. Here $G$ denotes the maximum $L_2$ norm of the feature vectors $\phi(x', y)$. By refining their analysis, [22] proved a $O(G^2/\lambda \epsilon)$ rate of convergence for a related but more general algorithm, which they called bundle methods for regularized risk minimization (BMRM). At first glance, it looks like the rates of convergence of these algorithms are independent of $|Y|$. This is somewhat misleading because, although the dependence is not direct, the convergence rates depend on $G$, which is in turn implicitly related to the size of $Y$.

Optimization algorithms which solve [7] in the dual have also been developed. For instance, the algorithm proposed by [7] performs exponentiated gradient descent in the dual and converges at $O\left(\frac{\log|Y|}{\lambda \epsilon}\right)$ rates. Again, these rates of convergence are not surprising given the well established lower bounds of [13] who show that, in general, non-smooth optimization problems cannot be solved in fewer than $\Omega(1/\epsilon)$ iterations by solvers which treat the objective function as a black box.

In this paper, we present an algorithm that provably converges to an $\epsilon$ accurate solution of [2] in $O\left(\sqrt{\frac{\log|Y|}{\lambda \epsilon}}\right)$ iterations. This does not contradict the lower bound because our algorithm is not a general purpose black box optimizer. In fact, it exploits the special form of the objective function [2]. Before launching into the technical details we would like to highlight some important features of our algorithm. First, compared to existing algorithms our convergence rates are better in terms of $|Y|$, $\lambda$, and $\epsilon$. Second, our convergence analysis is tighter in that our rates are with respect to the duality gap. Not only is the duality gap computable, it also upper bounds the primal and dual gaps used by other algorithms (see Figure 1). Finally, our cost per iteration is comparable with other algorithms.

To derive our algorithm we extend the recent excessive gap technique of [14] to Bregman projections and establish rates of convergence (Section 4). This extension is important because the original gradient based algorithm for strongly convex objectives by [14] does not admit graphical model factorizations, which are crucial for efficiency in structured prediction problems. We apply our resulting algorithm to the $M^N$ objective in Section 3. A straightforward implementation requires $O(|Y|)$ computational complexities per iteration, which makes it prohibitively expensive. We show that by exploiting the graphical model structure of $Y$ the cost per iteration can be reduced to $O(\log|Y|)$ (Section 4). Finally we contrast our algorithm with existing techniques in Section 5. The appendix contains some technical proofs and details on how to handle kernels.

2 Excessive Gap Technique with Bregman Projection

The following three concepts from convex analysis are extensively used in the sequel. Define $\mathbb{R} := \mathbb{R} \cup \{\infty\}$.

**Definition 1** A convex function $f : \mathbb{R}^n \to \overline{\mathbb{R}}$ is strongly convex with respect to a norm $\|\cdot\|$ if there exists a constant $\rho > 0$ such that $f - \frac{\rho}{2}\|\cdot\|^2$ is convex. $\rho$ is called the modulus of strong convexity of $f$, and for brevity we will call $f$ $\rho$-strongly convex.

**Definition 2** Suppose a function $f : \mathbb{R}^n \to \overline{\mathbb{R}}$ is differentiable on $Q \subseteq \mathbb{R}^n$. Then $f$ is said to have Lipschitz continuous gradient (l.c.g) with respect to a norm $\|\cdot\|$ if there exists a constant $L$ such that

$$\|\nabla f(w) - \nabla f(w')\| \leq L\|w - w'\| \quad \forall \ w, w' \in Q.$$  

For brevity, we will call $f$ $L$-l.c.g.

**Definition 3** The Fenchel dual of a function $f : \mathbb{R}^n \to \overline{\mathbb{R}}$ is a function $f^* : \mathbb{R}^n \to \overline{\mathbb{R}}$ defined by

$$f^*(w^*) = \sup_{w \in \mathbb{R}^n} \{\langle w, w^* \rangle - f(w)\}.$$  

Strong convexity and l.c.g are related by Fenchel duality according to the following lemma:

**Lemma 4** ([8, Theorem 4.2.1 and 4.2.2])

1. If $f : \mathbb{R}^n \to \overline{\mathbb{R}}$ is $\rho$-strongly convex, then $f^*$ is finite on $\mathbb{R}^n$ and $f^*$ is $\frac{1}{\rho}$-l.c.g.

2. If $f : \mathbb{R}^n \to \overline{\mathbb{R}}$ is convex, differentiable on $\mathbb{R}^n$, and $L$-l.c.g, then $f^*$ is $\frac{1}{L}$-strongly convex.

Let $Q_1$ and $Q_2$ be subsets of Euclidean spaces and $A$ be a linear map from $Q_1$ to $Q_2$. Suppose $f$ and $g$ are convex functions defined on $Q_1$ and $Q_2$ respectively. We are interested in the following optimization problem:

$$\min_{w \in Q_1} J(w) \quad \text{where} \quad J(w) := f(w) + g^*(Aw) = f(w) + \max_{\alpha \in Q_2} \{\langle Aw, \alpha \rangle - g(\alpha)\}.$$  


We will make the following standard assumptions: a) $Q_2$ is compact; b) with respect to a certain norm on $Q_1$, the function $f$ defined on $Q_1$ is $p$-strongly convex but not necessarily l.c.g, and c) with respect to a certain norm on $Q_2$, the function $g$ defined on $Q_2$ is $L_g$-l.c.g and convex, but not necessarily strongly convex. If we identify $f(w)$ with the regularizer and $g^*(Aw)$ with the loss function, then it is clear that (5) has the same form as (1) and (2). We will exploit this observation in Section 3.

The key difficulty in solving (5) arises because $g^*$ and hence $J$ may potentially be non-smooth. Our aim is to uniformly approximate $J(w)$ with a smooth and strongly convex function. Towards this end let $d$ be a $\sigma$ strongly convex smooth function with the following properties:

$$\min_{\alpha \in Q_2} d(\alpha) = 0, \quad \alpha_0 = \arg\min_{\alpha \in Q_2} d(\alpha), \quad \text{and} \quad D := \max_{\alpha \in Q_2} d(\alpha).$$

In optimization parlance, $d$ is called a prox-function. Let $\mu \in \mathbb{R}$ be an arbitrary positive constant, and

$$(g + \mu d)^\star(w) = \sup_{\alpha \in Q_2} \{\langle \alpha, w \rangle - g(\alpha) - \mu d(\alpha) \}. \quad (6)$$

If $D < \infty$ then it is easy to see that $(g + \mu d)^\star$ is uniformly close to $g^*$:

$$g^*(w) - \mu D \leq (g + \mu d)^\star(w) \leq g^*(w). \quad (7)$$

We will use $(g + \mu d)^\star$ to define a new objective function

$$J_\mu(w) := f(w) + (g + \mu d)^\star(Aw) = f(w) + \max_{\alpha \in Q_2} \{\langle Aw, \alpha \rangle - g(\alpha) - \mu d(\alpha) \}. \quad (8)$$

If some mild constraint qualifications hold [e.g. Theorem 3.3.5] one can write the dual $D(\alpha)$ of $J(w)$ using $A^\top$ (the transpose of $A$) as

$$D(\alpha) := -g(\alpha) - f^*(-A^\top \alpha) = -g(\alpha) - \max_{w \in Q_1} \{\langle -Aw, \alpha \rangle - f(w) \}, \quad (9)$$

and assert the following

$$\inf_{w \in Q_1} J(w) = \sup_{\alpha \in Q_2} D(\alpha), \quad \text{and} \quad J(w) \geq D(\alpha) \quad \forall \ w \in Q_1, \alpha \in Q_2. \quad (10)$$

The key idea of excessive gap minimization pioneered by [14] is to maintain two estimation sequences $\{w_k\}$ and $\{\alpha_k\}$, together with a diminishing sequence $\{\mu_k\}$ such that

$$J_{\mu_k}(w_k) \leq D(\alpha_k), \quad \text{and} \quad \lim_{k \to \infty} \mu_k = 0. \quad (11)$$

The idea is illustrated in Figure 2. In conjunction with (10) and (7), it is not hard to see that $\{w_k\}$ and $\{\alpha_k\}$ approach the solution of $\min_{w} J(w) = \max_{\alpha} D(\alpha)$. Using (7), (8), and (11), we can derive the rate of convergence of this algorithm:

$$J(w_k) - D(\alpha_k) \leq J_{\mu_k}(w_k) + \mu_k D - D(\alpha_k) \leq \mu_k D. \quad (12)$$

In other words, the duality gap is reduced at the same rate at which $\mu_k$ approaches 0. All that remains to turn this idea into an implementable algorithm is to answer the following two questions:

1. How to efficiently find initial points $w_1, \alpha_1$ and $\mu_1$ that satisfy (11).  
2. Given $w_k, \alpha_k$, and $\mu_k$, how to efficiently find $w_{k+1}, \alpha_{k+1}$, and $\mu_{k+1}$ which maintain (11).
Given a point \( \alpha \), the update rule of Algorithm 1 guarantees that Theorem 6. All that remains is to show that \( d \) based on Bregman projections, \( \mu \) is differentiable, we can define a Bregman divergence based on it:

\[
D(\alpha) := \langle A\alpha, \alpha \rangle - \langle A\alpha, \alpha \rangle - \langle \nabla d(\alpha), \alpha \rangle.
\]

To achieve the best possible convergence rate it is desirable to anneal \( \mu_k \) as fast as possible while still allowing \( w_k \) and \( \alpha_k \) to be updated efficiently. [14] gave a solution based on Euclidean projections, where \( \mu_k \) decays at \( 1/k^2 \) rate and all updates can be computed in closed form. We now extend his ideas to updates based on Bregman projections, which will be the key to our application to structured prediction problems later. Since \( d \) is differentiable, we can define a Bregman divergence based on it:

\[
\Delta(\hat{\alpha}, \alpha) := d(\hat{\alpha}) - d(\alpha) - \langle \nabla d(\alpha), \hat{\alpha} - \alpha \rangle.
\]

Given a point \( \alpha \) and a direction \( g \), we can define the Bregman projection as:

\[
V(\alpha, g) := \arg\min_{\hat{\alpha} \in Q_2} \{ \Delta(\hat{\alpha}, \alpha) + \langle g, \hat{\alpha} - \alpha \rangle \} = \arg\min_{\alpha \in Q_2} d(\hat{\alpha}) - \langle \nabla d(\alpha), g, \hat{\alpha} \rangle.
\]

Since \( f \) is assumed to be \( \rho \)-strongly convex, it follows from Lemma 4 that \(-D(\alpha)\) is l.c.g. If we denote its l.c.g modulus as \( L \), then an easy calculation [e.g. Eq. (7.2) [14]] shows that

\[
L = \frac{\|A\|^2}{\rho} + L_g, \quad \text{where } \|A\|_{1,2} := \max_{\|w\| = \|\alpha\| = 1} \langle A w, \alpha \rangle.
\]

For notational convenience, we define the following two maps:

\[
w(\alpha) := \arg\max_{w \in Q_1} \langle -A w, \alpha \rangle - f(w) = \nabla f^*(A\top \alpha),
\]

\[
\alpha_{\mu}(w) := \arg\max_{\alpha \in Q_2} \{ \langle A w, \alpha \rangle - g(\alpha) - \mu d(\alpha) \} = \nabla(g + \mu d)^*(A w).
\]

Since both \( f \) and \( (g + \mu d) \) are strongly convex, the above maps are unique and well defined. With this notation in place we now describe our excessive gap minimization method in Algorithm 1. Unrolling the recursive update for \( \mu_{k+1} \) yields

\[
\mu_{k+1} = (1 - \tau_k) \mu_k = \frac{k + 1}{k + 3} \mu_k = \frac{(k + 1)(k + 2) \ldots L}{(k + 3)(k + 2) \ldots 4} = \frac{6}{k + 3}\frac{L}{\sigma}.
\]

Plugging this into (12) and using (14) immediately yields a \( O(1/\sqrt{\epsilon}) \) rate of convergence of our algorithm:

**Theorem 5 (Rate of convergence for duality gap)** The sequences \( \{w_k\} \) and \( \{\alpha_k\} \) in Algorithm 1 satisfy

\[
J(w_k) - D(\alpha_k) \leq \frac{6LD}{\sigma(k + 1)(k + 2)} = \frac{6D}{\sigma(k + 1)(k + 2)} \left( \frac{\|A\|_{1,2}^2}{\rho} + L_g \right).
\]

All that remains is to show that

**Theorem 6** The update rule of Algorithm 1 guarantees that (11) is satisfied for all \( k \geq 1 \).

**Proof:** See Appendix A

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1 [14] did discuss updates based on Bregman projections, but just for the case where \( f \) is convex rather than strongly convex. Here, we show how to improve the convergence rate from \( O(1/\epsilon) \) to \( O(1/\sqrt{\epsilon}) \) when \( f \) is strongly convex.
Corollary 7 (Rate of convergence for dual gap) The sequence \( \{\alpha_k\} \) in Algorithm 1 satisfy
\[
\max_{\alpha \in Q_2} D(\alpha) - D(\alpha_k) \leq \frac{6 L d(\alpha^*)}{\sigma(k+1)(k+2)} = \frac{6 d(\alpha^*)}{\sigma(k+1)(k+2)} \left( \frac{\|A\|_{1,2}^2}{\rho} + L_g \right),
\]
where \( \alpha^* := \arg\max_{\alpha \in Q_2} D(\alpha) \). Note \( d(\alpha^*) \) is tighter than the \( D \) in (17).

Proof: See Appendix B.

3 Training Max-Margin Markov Networks

In the max-margin Markov network (M^3N) setting, we are given \( n \) labeled data points \( \{x^i, y^i\}_{i=1}^n \), where \( x^i \) are drawn from some space \( X \) and \( y^i \) belong to some space \( Y \). We assume that there is a feature map \( \phi \) which maps \((x, y)\) to a feature vector in \( \mathbb{R}^p \). Furthermore, for each \( x^i \), there is a label loss \( \ell^i_y := \ell(y^i, y^i; x^i) \) which quantifies the loss of predicting label \( y \) when the correct label is \( y^i \). Given this setup, the objective function minimized by M^3Ns can be written as
\[
J(w) = \frac{\lambda}{2} \|w\|^2 + \frac{1}{n} \sum_{i=1}^n \max_{y \in Y} \{\ell^i_y - \langle w, \psi^i_y \rangle\},
\]
where we used the shorthand \( \psi^i_y := \phi(x^i, y^i) - \phi(x^i, y) \). To write (19) in the form of (5), we define \( Q_1 = \mathbb{R}^p \), \( A \) to be a \( (n |Y|) \)-by-\( p \) matrix whose \((i,y)\)-th row is \((-\psi^i_y)^\top\),
\[
f(w) = \frac{\lambda}{2} \|w\|^2, \quad \text{and} \quad g^*(u) = \frac{1}{n} \sum_{y} \max_{i} \{\ell^i_y + u^i_y\}.
\]
Now, \( g \) can be verified to be:
\[
g(\alpha) = \begin{cases} -\sum_{i} \sum_{y \in Y} \ell^i_y \alpha^i_y & \text{if } \alpha^i_y \geq 0, \text{ and } \sum_{y} \alpha^i_y = \frac{1}{n}, \forall i \\ +\infty & \text{otherwise.} \end{cases}
\]
The domain of \( g \) is \( Q_2 = \mathbb{S}^n := \{\alpha \in [0,1]^{n|Y|} : \sum_{y} \alpha^i_y = \frac{1}{n}, \forall i \} \), which is convex and compact. Using the \( L_2 \) norm on \( Q_1 \) (i.e., \( \|w\| = \left( \sum_i w_i^2 \right)^{1/2} \)), \( f \) is clearly \( \lambda \)-strongly convex. Similarly, if we use the \( L_1 \) norm on \( Q_2 \) (i.e., \( \|\alpha\| = \sum_i \sum_{y} \alpha^i_y \)), then \( g \) is 0-l.c.g. By noting that \( f^*(-A^\top \alpha) = \frac{1}{2\lambda} \alpha^\top AA^\top \alpha \), one can write the dual form \( D(\alpha) : \mathbb{S}^n \mapsto \mathbb{R} \) of \( J(w) \) as
\[
D(\alpha) = -g(\alpha) - f^*(-A^\top \alpha) = -\frac{1}{2\lambda} \alpha^\top AA^\top \alpha + \sum_i \sum_{y} \ell^i_y \alpha^i_y, \quad \alpha \in \mathbb{S}^n. \tag{21}
\]

3.1 Rates of Convergence

A natural prox-function to use in our setting is the relative entropy with respect to the uniform distribution, which is defined as:
\[
d(\alpha) = \sum_{i=1}^n \sum_{y \in Y} \alpha^i_y \log \alpha^i_y + \log n + \log |Y|, \tag{22}
\]
Furthermore, \( d(\alpha) \leq D = \log |Y| \) for \( \alpha \in \mathbb{S}^n \), and the norm of \( A \) can be computed via
\[
\|A\|_{1,2} = \max_{w \in \mathbb{R}^p, u \in \mathbb{R}^{|Y|}} \left\{ \langle Aw , u \rangle : \sum_{i=1}^p u_i^2 = 1, \sum_{i=1}^n \sum_{y \in Y} |u^i_y| = 1 \right\} = \max_{i,y} \|\psi^i_y\|,
\]
where \( \|\psi^i_y\| \) is the Euclidean norm of \( \psi^i_y \). Since \( f \) is \( \lambda \)-strongly convex and \( L_g = 0 \), plugging this expression of \( \|A\|_{1,2} \) into (17) and (18), we obtain the rates of convergence for our algorithm:
\[
J(w_k) - D(\alpha_k) \leq \frac{6 \log |Y|}{(k+1)(k+2)} \max_{i,y} \|\psi^i_y\|^2 \quad \text{and} \quad \max_{\alpha \in Q_2} D(\alpha) - D(\alpha_k) \leq \frac{6 \KL(\alpha^*||\alpha_0)}{(k+1)(k+2)} \max_{i,y} \|\psi^i_y\|^2, \tag{23}
\]
where \( \KL(\alpha^*||\alpha_0) \) denotes the KL divergence between \( \alpha^* \) and the uniform distribution \( \alpha_0 \). Recall that for distributions \( p \) and \( q \) the KL divergence is defined as \( \KL(p||q) = \sum_i p_i \ln \frac{p_i}{q_i} \). Therefore to reduce the duality gap and dual gap below \( \epsilon \), it suffices to take the following number of steps respectively:
\[
\text{Duality gap: } 2 + \max_{i,y} \|\psi^i_y\| \sqrt{\frac{6 \log |Y|}{\lambda \epsilon}} \quad \text{Dual gap: } 2 + \max_{i,y} \|\psi^i_y\| \sqrt{\frac{6 \KL(\alpha^*||\alpha_0)}{\lambda \epsilon}}. \tag{23}
\]
3.2 Computing the Approximation \( J_\mu(w) \) and Connection to CRFs

In this section we show how to compute \( J_\mu(w) \). Towards this end, we first compute \((g + \mu d)^*(u)\).

**Lemma 8** The Fenchel dual of \((g + \mu d)\) is given by

\[
(g + \mu d)^*(u) = \frac{\mu}{n} \sum_{i=1}^{n} \log \sum_{y \in \mathcal{Y}} \exp \left( \frac{u_i^y + \ell_i^y}{\mu} \right) - \mu \log |\mathcal{Y}|, \tag{24}
\]

and the \((i, y)\)-th element of its gradient can be written as

\[
(\nabla (g + \mu d)^*(u))^i_y = \frac{1}{n} \exp \left( \frac{u_i^y + \ell_i^y}{\mu} \right) \right| \sum_{y'} \exp \left( \frac{u_i^{y'} + \ell_i^{y'}}{\mu} \right). \tag{25}
\]

**Proof:** See Supplementary Material \[\square\]

Using the above lemma, plugging in the definition of \( A \) and \( \psi^i_y \), and assuming that \( \ell_i^y \), = 0, we get

\[
J_\mu(w) = f(w) + (g + \mu d)^* (Aw) = \frac{\lambda}{2} \|w\|^2 - \frac{\mu}{n} \sum_{i=1}^{n} \log p(y^i|x^i; w) - \mu \log |\mathcal{Y}|, \tag{26}
\]

where \( p(y|x; w) \propto \exp \left( \frac{\ell^i_y + \langle w, \phi(x^i, y) \rangle}{\mu} \right) \).

This interpretation clearly shows that the approximation \( J_\mu(w) \) essentially converts the maximum margin estimation problem \[\square\] into a CRF estimation problem \[\square\]. Here \( \mu \) determines the quality of the approximation; when \( \mu \rightarrow 0 \), \( p(y|x; w) \) tends to the delta distribution with the probability mass concentrated on \( \text{argmax}_y \ell^i_y + \langle w, \phi(x^i, y) \rangle \). Besides, the loss \( \ell^i_y \) rescales the distribution.

Given the above interpretation, it is tempting to argue that every non-smooth problem can be solved by computing a smooth approximation \( J_\mu(w) \), and applying a standard smooth convex optimizer to minimize \( J_\mu(w) \). Unfortunately, this approach is fraught with problems. In order to get a close enough approximation of \( J(w) \) the \( \mu \) needs to be set to a very small number which makes \( J_\mu(w) \) ill-conditioned and leads to numerical issues in the optimizer. The excessive gap technique adaptively changes the \( \mu \) in each iteration in order to avoid these problems.

4 Efficient Implementation by Exploiting Clique Decomposition

In the structured large margin setting, the number of labels \(|\mathcal{Y}|\) could potentially be exponentially large. For example, if a sequence has \( l \) nodes and each node has two states, then \(|\mathcal{Y}| = 2^l\). A naive implementation of the excessive gap reduction algorithm described in the previous section requires maintaining and updating \( O(|\mathcal{Y}|) \) coefficients at every iteration, which is prohibitively expensive. With a view to reducing the computational complexity, and also to take into account the inherent conditional independence properties of the output space, it is customary to assume that \( \mathcal{Y} \) is endowed with a graphical model structure; we refer the reader to \[\square\] for an in-depth treatment of this issue. For our purposes it suffices to assume that \( \ell(y, y'; x^i) \) and \( \phi(x^i, y) \) decompose according to the cliques\(^3\) of an undirected graphical model, and hence can be written (with some abuse of notation) as

\[
\ell^i_y = \ell(y, y'; x^i) = \sum_{c \in \mathcal{C}} \ell(y_c, y'_c; x^i) = \sum_{c \in \mathcal{C}} \ell^i_{y_c}, \quad \phi(x^i, y) = \oplus_{c \in \mathcal{C}} \phi(x^i, y_c), \text{ and } \psi^i_y = \oplus_{c \in \mathcal{C}} \psi^i_{y_c}. \tag{27}
\]

Here \( \mathcal{C} \) denotes the set of all cliques of the graphical model and \( \oplus \) denotes vector concatenation. More explicitly, \( \psi^i_{y_c} \) is the vector on the graphical model obtained by accumulating the vector \( \psi^i_{y_c} \) on all the cliques \( c \) of the graph.

Let \( h_c(y_c) \) be an arbitrary real valued function on the value of \( y \) restricted to clique \( c \). Graphical models define a distribution \( p(y) \) on \( y \in \mathcal{Y} \) whose density takes the following factorized form:

\[
p(y) \propto q(y) = \prod_{c \in \mathcal{C}} \exp (h_c(y_c)). \tag{28}
\]

The key advantage of a graphical model is that the marginals on the cliques can be efficiently computed:

\[
m_{y_c} := \sum_{z | z_c = y_c} q(z) = \sum_{z | z_c = y_c} \prod_{c' \in \mathcal{C}} \exp (h_{c'}(z_{c'})).
\]

\(^3\)Any fully connected subgraph of a graph is called a clique.
where the summation is over all the configurations $z$ in $\mathcal{Y}$ whose restriction on the clique $c$ equals $y_c$. Although $\mathcal{Y}$ can be exponentially large, efficient dynamic programming algorithms exist that exploit the factorized form \[25\], e.g. belief propagation \[11\]. The computational cost is $O(s^n)$ where $s$ is the number of states of each node, and $\omega$ is the maximum size of the cliques. For example, a linear chain has $\omega = 2$. When $\omega$ is large, approximate algorithms also exist \[24\][2][9]. In the sequel we will assume that our graphical models are tractable, i.e., $\omega$ is low.

### 4.1 Basics

At each iteration of Algorithm\[1\] we need to compute four quantities: $w(\alpha), \nabla D(\alpha), \alpha_{i,c}(w)$, and $V(\alpha, g)$.

Below we rewrite them by taking into account the factorization \[27\], and postpone to Section 4.2 the discussion on how to compute them efficiently. Since $\alpha^i_Y \geq 0$ and $\sum_y \alpha^i_Y = \frac{1}{\lambda}$, the $\{\alpha^i_Y : y \in \mathcal{Y}\}$ form an unnormalized distribution, and we denote its (unnormalized) marginal distribution on clique $c$ by

$$\alpha^i_y := \sum_{z|z|_c = y_c} \alpha^i_z.$$  

(29)

The feature expectations on the cliques with respect to the unnormalized distributions $\alpha$ are important:

$$\mathbb{E}[\psi^i_{yc} ; \alpha] := \sum_{y_c} \alpha^i_{yc} \psi^i_{yc}$$

and

$$\mathbb{E}[\psi_{yc} ; \alpha] := \sum_i \mathbb{E}[\psi^i_{yc} ; \alpha].$$

(30)

Clearly, if for all $i$ the marginals of $\alpha$ on the cliques (i.e., $\{\alpha^i_{yc} : i, c, y_c\}$ in (29)) are available, then these two expectations can be computed efficiently.

- **$w(\alpha)$**: As a consequence of (27), we can write $\psi^i_Y = \psi^i_Y$. Plugging this into (15a) and recalling that $\nabla f^\ast(-A^\top \alpha) = \frac{1}{\lambda} A^\top \alpha$ yields the following expression for $w(\alpha) = \frac{1}{\lambda} A^\top \alpha$:

$$w(\alpha) = \frac{1}{\lambda} \sum_i \sum_y \alpha^i_Y \psi^i_Y = \frac{1}{\lambda} \sum_i \sum_y \alpha^i_Y \left( \psi^i_Y \right) = \frac{1}{\lambda} \sum_i \mathbb{E}[\psi^i_{yc} ; \alpha] = \frac{1}{\lambda} \sum_{c} \mathbb{E}[\psi_{yc} ; \alpha].$$

(31)

- **$\nabla D(\alpha)$**: Using (21) and the definition of $w(\alpha)$, the $(i,y)$-th element of $\nabla D(\alpha)$ can be written as

$$\left( \nabla D(\alpha) \right)^i_y = \ell^i_y - \frac{1}{\lambda} \left( AA^\top \alpha \right)^i_y = \ell^i_y - \left( \psi^i_Y, w(\alpha) \right) = \sum_c \left( \ell^i_{yc} - \frac{1}{\lambda} \left( \psi^i_{yc}, \mathbb{E}[\psi_{yc} ; \alpha] \right) \right).$$

(32)

- **$\alpha_{\mu}(w)$**: Using (15b) and (25), the $(i,y)$-th element of $\alpha_{\mu}(w)$ given by $\left( (g + \mu d)^\ast(Aw) \right)^i_y$ can be written as

$$\left( \alpha_{\mu}(w) \right)^i_y = \frac{1}{\eta} \exp \left( \mu^{-1} \left( \ell^i_y - \langle \psi^i_Y, w \rangle \right) \right) = \frac{1}{\eta} \sum_{y'} \exp \left( \mu^{-1} \left( \ell^i_{y'} - \langle \psi^i_{y'}, w \rangle \right) \right).$$

(33)

- **$V(\alpha, g)$**: Since the prox-function $d$ is the relative entropy, the $(i,y)$-th element of $V(\alpha, g)$ is

$$\left( V(\alpha, g) \right)^i_y = \frac{1}{\eta} \alpha^i_{yc} \exp(-g_{yc}).$$

(34)

### 4.2 Efficient Computation

We now show how the algorithm can be made efficient by taking into account \[27\]. Key to our efficient implementation are the following four observations from Algorithm \[1\] when applied to the structured large margin setting. In particular, we will exploit the fact that the marginals of $\alpha_k$ can be updated iteratively.

- **The marginals of $\alpha_{\mu_k}(w_k)$ and $\hat{\alpha}$ can be computed efficiently**. From (33) it is easy to see that $\alpha_{\mu_k}(w_k)$ can be written as a product of factors over cliques, that is, in the form of \[28\]. Therefore, the marginals of $\alpha_{\mu_k}(w_k)$ can be computed efficiently. As a result, if we keep track of the marginal distributions of $\alpha_k$, then it is trivial to compute the marginals of $\hat{\alpha} = (1 - \tau_k)\alpha_k + \tau_k \alpha_{\mu_k}(w_k)$.

- **The marginals of $\alpha$ can be computed efficiently**. Define $\eta = \frac{-\tau_k}{(1-\tau_k)\mu_k}$. By plugging in (32) and (33) into (34) and observing that $\nabla D(\alpha)$ can be written as a sum of terms over cliques obtains:

$$\hat{\alpha}^i_Y = \left( V(\alpha_{\mu_k}(w_k), \eta \nabla D(\hat{\alpha})) \right)^i_Y \times \left( \alpha_{\mu_k}(w_k) \right)^i_Y \exp \left( -\eta \left( \nabla D(\hat{\alpha}) \right)^i_Y \right)$$

$$= \prod_c \exp \left( \mu_k^{-1} \left( \ell^i_{yc} - \langle \psi^i_{yc}, (w_k) \rangle \right) \right) - \eta \ell^i_{yc} + \eta \lambda^{-1} \left( \psi^i_{yc}, \mathbb{E}[\psi_{yc} ; \hat{\alpha}] \right).$$

(35)

Clearly, $\hat{\alpha}$ factorizes and has the form of \[28\]. Hence its marginals can be computed efficiently.
technically such factorizations are not applicable to projected gradient. Second, we designed a nontrivial
based updates in excessive gap optimization, while [14] showed this rate only for projected gradient style
products can be evaluated via kernels on the cliques:
\[ \phi \]

4.3 Kernelization

and dual objectives
\[ J, \]

implementation can be sped up in many ways. The last issue to be addressed is the computation of the primal
\[ M, \]

for concreteness, let us consider a sequence as an example. Here the cliques are just edges between consec-

4.4 Efficiency in Memory and Computation

\[
\text{Algorithm 2: Max-margin structured learning using clique factorization}
\]

\[
\text{Input: Loss functions \( \{ l^j_x \} \) and features \( \{ \psi^j_x \} \), a regularization parameter \( \lambda \), a tolerance level \( \epsilon > 0 \).
}\]

\[
\text{Output: A pair \( w \) and \( \alpha \) that satisfy } J(w) - D(\alpha) < \epsilon.
]\]

\[
1 \quad \text{Initialize: } k \leftarrow 1, \mu_1 \leftarrow \lambda \max_{i,y} \left\| \psi^j_y \right\|^2, \alpha_0 \leftarrow \left( \frac{1}{n|\mathcal{Y}|}, \ldots, \frac{1}{n|\mathcal{Y}|} \right) \trans \in \mathbb{R}^{|\mathcal{Y}|};
\]

\[
2 \quad \text{Update } w_1 \leftarrow w(\alpha_0) = \frac{1}{n} \sum_{c \in \mathcal{C} } \mathbb{F}[\psi^c; \alpha_0]., \alpha_1 \leftarrow V \left( \alpha_0, -\frac{1}{\mu_1} \nabla D(\alpha_0) \right) \text{ and compute its marginals.};
\]

\[
3 \quad \text{while } J(w_k) - D(\alpha_k) \geq \epsilon \text{ do } / \star \text{ Termination criteria: duality gap falls below } \epsilon \text{ */}
\]

\[
4 \quad \tau_k \leftarrow \epsilon + \frac{1}{\sqrt{k}};\quad ;
\]

\[
5 \quad \text{Compute the marginals of } \alpha_{\mu_k}(w_k) \text{ by exploiting (33).} ;
\]

\[
6 \quad \text{for all the cliques } c \in \mathcal{C} \text{ do}
\]

\[
7 \quad \text{Compute the marginals } \tilde{\alpha}_c \text{ by convex combination: } \tilde{\alpha}_c \leftarrow (1 - \tau_k)(\tilde{\alpha}_c) + \tau_k(\alpha_{\mu_k}(w_k))_c;\quad ;
\]

\[
8 \quad \text{Update the weight on clique } c: \quad (w_{k+1})_c \leftarrow (1 - \tau_k)(w_k)_c + \tau_k \alpha_{\mu_k}(w_k)_c ;
\]

\[
9 \quad \text{Compute the marginals of } \tilde{\alpha} \text{ by exploiting (35) and using the marginals } \{ \tilde{\alpha}_c \};
\]

\[
10 \quad \text{for all the cliques } c \in \mathcal{C} \text{ do}
\]

\[
11 \quad \text{Update the marginals } (\alpha_k)_c \text{ by convex combination: } \quad (\alpha_{k+1})_c \leftarrow (1 - \tau_k)(\alpha_k)_c + \tau_k \tilde{\alpha}_c ;
\]

\[
12 \quad \text{Update } \mu_{k+1} \leftarrow (1 - \tau_k)(\mu_k), \quad k \leftarrow k + 1.;
\]

\[
13 \quad \text{return } w_k \text{ and } \alpha_k.;
\]

- The marginals of \( \alpha_k \) can be updated efficiently. Given the marginals of \( \tilde{\alpha} \), it is trivial to update the marginals of \( \alpha_{k+1} \) since \( \alpha_{k+1} = (1 - \tau_k)\alpha_k + \tau_k \tilde{\alpha} \). For convenience, define \( \alpha_c := \{ \alpha^c_{y_c}; i, y_c \} \).

- \( w_k \) can be updated efficiently. According to step 5 of Algorithm 1 by using (31) we have
\[
(w_{k+1})_c = (1 - \tau_k)(w_k)_c + \tau_k \alpha_{\mu_k}(w_k)_c = (1 - \tau_k)(w_k)_c + \tau_k \lambda^{-1} \mathbb{F}[\psi^c; \tilde{\alpha}].
\]

Leveraging these observations, Algorithm 2 provides a complete listing of how to implement the excessive
gap technique with Bregman projections for training M3N. It focuses on clarifying the ideas; a practical
implementation can be sped up in many ways. The last issue to be addressed is the computation of the primal
and dual objectives \( J(w_k) \) and \( D(\alpha_k) \), so as to monitor the duality gap. See Appendix C for details.

4.3 Kernelization

When nonlinear kernels are used, the feature vectors \( \phi^j_x \) are not expressed explicitly and only their inner
products can be evaluated via kernels on the cliques:
\[
\langle \psi^i_y, \psi^j_y \rangle := k((x^i, y), (x^j, y')) = \sum_c k_c((x^i, y_c), (x^j, y'_c)), \quad \text{where } k_c((x^i, y_c), (x^j, y'_c)) := \langle \psi^i_{y_c}, \psi^j_{y'_c} \rangle.
\]

Algorithm 2 is no longer applicable because no explicit expression of \( w \) is available. However, by rewriting
\( w \) as the feature expectations with respect to some underlying distribution which can be updated implicitly,
all the updates and objective function evaluations can still be done efficiently. Details are in Appendix D.

4.4 Efficiency in Memory and Computation

For concreteness, let us consider a sequence as an example. Here the cliques are just edges between consec-
utive nodes. Suppose there are \( l + 1 \) nodes and each node has \( s \) states. The memory cost of Algorithm 2 is
\( O(nls^2) \), due to the storage of the marginals. The computational cost per iteration is dominated by calculating
the marginals of \( \alpha \) and \( \tilde{\alpha} \), which is \( O(nls^2) \) by standard graphical model inference. The rest operations in
Algorithm 2 cost \( O(nls^2) \) for linear kernels. If nonlinear kernels are used, then the cost becomes \( O(n^2ls^2) \)
(see Appendix D).

5 Discussion

Structured output prediction is an important learning task in both theory and practice. The main contribution
of our paper is two fold. First, we identified an efficient algorithm by [14] for solving the optimization
problems in structured prediction. We proved the \( O(1/\sqrt{\epsilon}) \) rate of convergence for the Bregman projection
based updates in excessive gap optimization, while [14] showed this rate only for projected gradient style
updates. In M3N optimization, Bregman projection plays a key role in factorizing the computations, while
technically such factorizations are not applicable to projected gradient. Second, we designed a nontrivial
application of the excessive gap technique to M^3N optimization, in which the computations are kept efficient by using the graphical model decomposition. Kernelized objectives can also be handled by our method, and we proved superior convergence and computational guarantees than existing algorithms.

When M^3Ns are trained in a batch fashion, we can compare the convergence rate of dual gap between our algorithm and the exponentiated gradient method [ExpGrad, 7]. Assume \( \alpha_0 \), the initial value of \( \alpha \), is the uniform distribution and \( \alpha^* \) is the optimal dual solution. Then by (23), we have

\[
\text{Ours: } \max_{i,y} \left\| \psi^i_y \right\| \sqrt{\frac{6KL(\alpha^* || \alpha^0)}{\lambda \epsilon}}, \quad \text{ExpGrad: } \max_{i,y} \left\| \psi^i_y \right\| \frac{2KL(\alpha^* || \alpha^0)}{\lambda \epsilon}.
\]

It is clear that our iteration bound is almost the square root of ExpGrad, and has much better dependence on \( \epsilon, \lambda, \max_{i,y} \left\| \psi^i_y \right\| \), as well as the divergence from the initial guess to the optimal solution \( KL(\alpha^* || \alpha^0) \).

In addition, the cost per iteration of our algorithm is almost the same as ExpGrad, and both are governed by the computation of the expected feature values on the cliques (which we call exp-oracle), or equivalently the marginal distributions. For graphical models, exact inference algorithms such as belief propagation can compute the marginals via dynamic programming [11]. Finally, although both algorithms require marginalization, they are calculated in very different ways. In ExpGrad, the dual variables \( \alpha \) correspond to a factorized distribution, and in each iteration its potential functions on the cliques are updated using the exponentiated gradient rule. In contrast, our algorithm explicitly updates the marginal distributions of \( \alpha_k \) on the cliques, and marginalization inference is needed only for \( \alpha \) and \( \tilde{\alpha} \). Indeed, the joint distribution \( \alpha \) does not factorize, which can be seen from step 7 of Algorithm 1. The convex combination of two factorized distributions is not necessarily factorized.

Marginalization is just one type of query that can be answered efficiently by graphical models, and another important query is the max a-posteriori inference (which we call max-oracle): given the current model \( w \), find the argmax in \( \mathcal{Y} \). Max-oracle has been used by greedy algorithms such as cutting plane (BMRM and SVM-Struct) and sequential minimal optimization [SMO, 17, Chapter 6]. SMO picks the steepest descent coordinate in the dual and greedily optimizes the quadratic analytically, but its convergence rate is slower than BMRM by a factor \( n \). The max-oracle again relies on graphical models for dynamical programming [9], and many existing combinatorial optimizers can also be used, such as in the applications of matching [21] and context free grammar parsing [19]. Furthermore, this oracle is particularly useful for solving the slack rescaling variant of M^3N proposed by [23]:

\[
J(w) = \frac{\lambda}{2} \left\| w \right\|^2 + \frac{1}{n} \sum_{i=1}^{n} \max_{y \in \mathcal{Y}} \left\{ \ell(y, y^i; x^i) \left( 1 - \langle w, \phi(x^i, y^i) - \phi(x^i, y) \rangle \right) \right\}.
\]

Here two factorized terms get multiplied, which causes additional complexity in finding the maximizer. [1] Section 1.4.1] solved this problem by a modified dynamic program. Nevertheless, it is not clear how ExpGrad or our method can be used to optimize this objective.

In the quest for faster optimization algorithms for M^3Ns, the following three questions are important: how hard is it to optimize M^3N intrinsically, how informative is the oracle which is the only way for the algorithm to access the objective function, and how well does the algorithm make use of such information. The superiority of our algorithm suggests that the exp-oracle is more informative than the max-oracle, and a deeper explanation is that the max-oracle is local while the exp-oracle is not [13] Section 1.3. Hence there is no surprise that the less informative max-oracle is easier to compute, which makes it applicable to a wider range of problems such as (35). Moreover, the comparison between ExpGrad and our algorithm shows that even if the exp oracle is used, the algorithm still needs to make good use of it in order to converge faster.

For future research, it is interesting to study the lower bound complexity for optimizing M^3N, including the dependence on \( \epsilon, n, \lambda, \mathcal{Y} \), and probably even on the graphical model topology. Empirical evaluation of our algorithm is also desirable, along the lines of sequence labeling, word alignment, context free grammar parsing, etc.

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Appendix (to be considered in the 13 page limit)

A Proof of Theorem

To prove Theorem, we begin with a technical lemma.

Lemma 9 (Lemma 7.2 of [14]) For any \( \alpha \) and \( \bar{\alpha} \), we have

\[
D(\alpha) + \langle \nabla D(\alpha), \bar{\alpha} - \alpha \rangle \geq -g(\bar{\alpha}) + \langle A w(\alpha), \bar{\alpha} \rangle + f(w(\alpha)).
\]
**Proof:** Direct calculation by plugging in (15a) into (9) and using the convexity of $g$ yields
\[
D(\alpha) + \langle \nabla D(\alpha), \alpha - \alpha \rangle = -g(\alpha) + \langle Aw(\alpha), \alpha \rangle + f(w(\alpha)) + \langle -\nabla g(\alpha) + Aw(\alpha), \alpha - \alpha \rangle \\
\geq -g(\alpha) + \langle Aw(\alpha), \alpha \rangle + f(w(\alpha)).
\]

Furthermore, because $d$ is $\sigma$-strongly convex, it follows that
\[
\Delta(\alpha, \alpha) = d(\alpha) - d(\alpha) - \langle \nabla d(\alpha), \alpha - \alpha \rangle \geq \frac{\sigma}{2} \| \alpha - \alpha \|^2.
\]

As $\alpha_0$ minimizes $d$ over $Q_2$, we have
\[
\langle \nabla d(\alpha_0), \alpha - \alpha_0 \rangle \geq 0 \quad \forall \alpha \in Q_2.
\]

We first show that the initial $w_1$ and $\alpha_1$ satisfy the excessive gap condition (11). Since $-D$ is $L$-L.c.g., so
\[
D(\alpha_1) \geq D(\alpha_0) + \langle \nabla D(\alpha_0), \alpha_1 - \alpha_0 \rangle - \frac{1}{2} L \| \alpha_1 - \alpha_0 \|^2
\]
(using defn. of $\mu_1$ and (17))
\[
\geq D(\alpha_0) + \langle \nabla D(\alpha_0), \alpha_1 - \alpha_0 \rangle - \mu_1 \Delta(\alpha_1, \alpha_0)
\]
(using defn. of $\alpha_1$)
\[
= \max_{\alpha \in Q_2} \{ D(\alpha_0) + \langle \nabla D(\alpha_0), \alpha - \alpha_0 \rangle - \mu_1 d(\alpha) \}
\]

\[
\geq \max_{\alpha \in Q_2} \{ -g(\alpha) + \langle Aw(\alpha_0), \alpha \rangle + f(w(\alpha_0)) - \mu_1 d(\alpha) \}
\]

which shows that our initialization indeed satisfies (11). Second, we prove by induction that the updates in Algorithm 1 maintain (11). We begin with two useful observations. Using (16) and the definition of $\tau_k$, one can bound
\[
\mu_{k+1} = \frac{6}{(k+3)(k+2)} \geq \frac{3L}{2}. \tag{39}
\]

Let $\beta := \alpha_{\mu_2}(w_k)$. The optimality conditions for (15b) imply
\[
\langle \mu_k \nabla d(\beta) - Aw_k + \nabla g(\beta), \alpha - \beta \rangle \geq 0. \tag{40}
\]

By using the update equation for $w_{k+1}$ and the convexity of $f$
\[
J_{\mu_{k+1}}(w_{k+1}) = f(w_{k+1}) + \max_{\alpha \in Q_2} \{ \langle Aw_{k+1}, \alpha \rangle - g(\alpha) - \mu_{k+1} d(\alpha) \}
\]
\[
= f((1-\tau_k)w_k + \tau_k w(\alpha)) + \max_{\alpha \in Q_2} \{ (1-\tau_k) \langle Aw_k, \alpha \rangle + \tau_k \langle Aw(\alpha), \alpha \rangle - g(\alpha) - (1-\tau_k)\mu_k d(\alpha) \}
\]
\[
\leq \max_{\alpha \in Q_2} \{ (1-\tau_k) T_1 + \tau_k T_2 \},
\]

where $T_1 = [-\mu_k d(\alpha) + \langle Aw_k, \alpha \rangle - g(\alpha) + f(w_k)]$ and $T_2 = [-g(\alpha) + \langle Aw(\alpha), \alpha \rangle + f(w(\alpha))]$.

$T_1$ can be bounded as follows
\[
T_1 = -\mu_k d(\alpha) + \langle Aw_k, \alpha \rangle - g(\alpha) + f(w_k)
\]
(using defn. of $\Delta$)
\[
\leq -\mu_k \Delta(\alpha, \beta) - \mu_k d(\beta) + \langle Aw_k + \nabla g(\beta), \alpha - \beta \rangle + \langle Aw_k, \alpha \rangle - g(\alpha) + f(w_k)
\]
(using (40))
\[
= -\mu_k \Delta(\alpha, \beta) - \mu_k d(\beta) + \langle Aw_k, \beta \rangle - g(\beta) + \langle \nabla g(\beta), \alpha - \beta \rangle + f(w_k)
\]
(using convexity of $g$)
\[
= -\mu_k \Delta(\alpha, \beta) - \mu_k d(\beta) + \langle Aw_k, \beta \rangle - g(\beta) + f(w_k)
\]
(using defn. of $\beta$)
\[
= -\mu_k \Delta(\alpha, \beta) + D(\alpha_k)
\]
(assuming induction assumption)
\[
\leq -\mu_k \Delta(\alpha, \beta) + D(\alpha_k)
\]
(assuming concavity of $D$)

while $T_2$ can be bounded by using Lemma [9]
\[
T_2 = -g(\alpha) + \langle Aw(\alpha), \alpha \rangle + f(w(\alpha)) \leq D(\alpha) + \langle \nabla D(\alpha), \alpha - \alpha \rangle.
\]
Putting the upper bounds on $T_1$ and $T_2$ together, we obtain the desired result.

\[
J_{\mu k+1}(w_{k+1}) \leq \max_{\alpha \in Q_2} \{ (1 - \tau_k) \left[ -\mu_k \Delta(\alpha, \beta) + D(\hat{\alpha}) + \langle \nabla D(\hat{\alpha}), \alpha_k - \hat{\alpha} \rangle \right] + \tau_k \left[ D(\hat{\alpha}) + \langle \nabla D(\hat{\alpha}), \alpha - \hat{\alpha} \rangle \right] \}
\]

\[
= \max_{\alpha \in Q_2} \{ -\mu_k \Delta(\alpha, \beta) + D(\hat{\alpha}) + \langle \nabla D(\hat{\alpha}), (1 - \tau_k) \alpha_k + \tau_k \alpha - \hat{\alpha} \rangle \}
\]

(Using defn. of $\hat{\alpha}$)

\[
= \max_{\alpha \in Q_2} \{ -\mu_k \Delta(\alpha, \beta) + D(\hat{\alpha}) + \langle \nabla D(\hat{\alpha}), \alpha - \beta \rangle \}
\]

(Using defn. of $\hat{\alpha}$)

\[
= -\min_{\alpha \in Q_2} \{ \mu_k \Delta(\alpha, \beta) - D(\hat{\alpha}) - \tau_k \langle \nabla D(\hat{\alpha}), \alpha - \beta \rangle \}
\]

(Using defn. of $\alpha_{k+1}$)

\[
= -\frac{1}{2} \tau_k^2 L \| \alpha - \beta \|^2 + D(\hat{\alpha}) + \tau_k \langle \nabla D(\hat{\alpha}), \alpha - \beta \rangle
\]

(by $L$-l.c.g of $-D$) \leq D(\alpha_{k+1}).

**B Proof of Corollary 7**

\[
D(\alpha_{k+1}) \geq J_{\mu k+1}(w_{k+1}) = f(w_{k+1}) + \max_{\alpha} \{ \langle Aw_{k+1}, \alpha \rangle - g(\alpha) - \mu_{k+1}d(\alpha) \}
\]

\[
\geq f(w_{k+1}) + \langle Aw_{k+1}, \alpha^* \rangle - g(\alpha^*) - \mu_{k+1}d(\alpha^*)
\]

\[
\geq -g(\alpha^*) + \min_w \{ f(w) + \langle Aw, \alpha^* \rangle \} - \mu_{k+1}d(\alpha^*)
\]

\[
= D(\alpha^*) - \mu_{k+1}d(\alpha^*).
\]

**C Primal and Dual Objective Evaluation using Clique Decomposition**

We show how to efficiently compute the primal and dual objective function values. The primal objective value is easy due to the convenience in computing $\|w_k\|^2$ and inner products between $w_k$ and feature vectors. Afterwards any MAP algorithm can be used to find the $\max_{\mathcal{Y}}$. The dual objective $\|D(\alpha_k)\|$ is also easy since

\[
\sum \sum \ell(y) (\alpha_k)_y = \sum \sum \ell(y) (\alpha_k)_y = \sum \sum \ell(y) (\alpha_k)_y = \sum \ell(y) (\alpha_k)_y,
\]

and the marginals of $\alpha_k$ are available. Finally, the quadratic term in $D(\alpha_k)$ can be computed as follows.

\[
\|A^T \alpha_k\|^2 = \left\| \sum \sum \psi(y) (\alpha_k)_y \right\|^2 = \sum \sum \sum \psi(y) (\alpha_k)_y = \sum \sum \psi(y) (\alpha_k)_y = \sum \psi(y) (\alpha_k)_y
\]

where the inner term is the same as the unnormalized expectation that can be efficiently calculated. The last formula is only for nonlinear kernels.

**D Kernelizing the Excessive Gap Method for M3Ns**

Compared with the linear kernel case, the only difficulty caused by nonlinear kernels is that the $w_k$ cannot be expressed explicitly. However, if $w_k$ can be expressed as the expectation of the feature vector with respect to some distribution $\beta_k \in S^n$, then we only need to update $w_k$ implicitly via $\beta_k$, and the inner product between $w_k$ and any feature vector can also be efficiently calculated. We formalize and prove this claim by induction.

**Theorem 10** For all $k \geq 0$, there exists $\beta_k \in S^n$, such that $(w_k)_c = \frac{1}{\lambda} \mathbb{E}[\psi_c; \beta_k]$ and $\beta_k$ can be updated by

\[
\beta_{k+1} = (1 - \tau_k) \beta_k + \tau_k \hat{\alpha}_k.
\]

**Proof:** First, $w_1 = w(\alpha_0) = \frac{1}{\lambda} \mathbb{E}[\psi_c; \alpha_0]$, so $\beta_1 = \alpha_0$. Suppose the claim holds for all $1, \ldots, k$, then

\[
(w_{k+1})_c = (1 - \tau_k) (w_k)_c + \frac{\tau_k}{\lambda} \mathbb{E}[\psi_c; (\hat{\alpha}_k)_c] = (1 - \tau_k) \frac{1}{\lambda} \mathbb{E}[\psi_c; \beta_k] + \frac{\tau_k}{\lambda} \mathbb{E}[\psi_c; (\hat{\alpha}_k)_c]
\]

\[
= \frac{1}{\lambda} \mathbb{E}[\psi_c; (1 - \tau_k) (\beta_k)_c + \tau_k (\hat{\alpha}_k)_c].
\]

Therefore, we can set $\beta_{k+1} = (1 - \tau_k) \beta_k + \tau_k \hat{\alpha}_k \in S^n$.  \[\blacksquare\]
In general $\alpha_k \neq \tilde{\alpha}_k$, hence $\beta_k \neq \alpha_k$. To compute $\langle \psi^i_{y_c}, (w_k)_c \rangle$ required by (35), we have

$$\langle \psi^i_{y_c}, (w_k)_c \rangle = \left\langle \psi^i_{y_c}, \frac{1}{\lambda} \sum_j \sum_{y_c'} \beta^i_{y_c} \psi^j_{y_c'} \right\rangle = \frac{1}{\lambda} \sum_j \sum_{y_c'} \beta^i_{y_c} k_c((x^i, y_c), (x^j, y_c')).$$

And by using this trick, all the iterative updates in Algorithm 2 can be done efficiently. So is the evaluation of $\|w_k\|^2$ and the primal and dual objectives. We leave the details to the reader.
E Proof of Lemma

Proof: Using (20) and (22) we can write
\[
(g + ud)^*(u) = \sup_{\alpha \in \mathcal{S}^n} \{ \langle u, \alpha \rangle - g(\alpha) - \mu d(\alpha) \}
\]
\[
= \sup_{\alpha \in \mathcal{S}^n} \sum_i \sum_y u_i^y \alpha_i^y + \sum_i \sum_y \ell_i^y \alpha_i^y - \mu \sum_i \sum_y \alpha_i^y \log \alpha_i^y - \mu \log n - \mu \log |\mathcal{Y}|
\]
\[
= \sup_{\alpha \in \mathcal{S}^n} \sum_i \sum_y (u_i^y + \ell_i^y - \mu \log \alpha_i^y)\alpha_i^y - \mu \log n - \mu \log |\mathcal{Y}|
\]

By introducing non-negative Lagrange multipliers \(\sigma_i\) we can write the partial Lagrangian of the above maximization problem:
\[
L(\alpha, \sigma) = \sup_{\alpha \in \mathcal{S}^n} \sum_i \sum_y (u_i^y + \ell_i^y - \mu \log \alpha_i^y)\alpha_i^y - \mu \log n - \mu \log |\mathcal{Y}| - \sum_i \sigma_i \left( \sum_y \alpha_i^y - \frac{1}{n} \right).
\]

Taking partial derivative with respect \(\alpha_i^y\) and setting it to 0, we get
\[
u_i^y + \ell_i^y - \mu \log \alpha_i^y - \mu - \sigma_i = 0.
\]
Therefore
\[
\alpha_i^y = \exp \left( \frac{u_i^y + \ell_i^y}{\mu} \right), \quad \text{where} \ Z_i := \sum_y \exp \left( \frac{u_i^y + \ell_i^y}{\mu} \right).
\]

Plugging this back to the Lagrangian, we can eliminate both \(\alpha\) and \(\sigma\), and write out the solution of the optimization problem in closed form
\[
\sum_{i,y} (\mu \log Z_i + \mu \log n)\alpha_i^y - \mu \log n - \mu \log |\mathcal{Y}| = \frac{\mu}{n} \sum_{i=1}^n \log \sum_{y \in \mathcal{Y}} \exp \left( \frac{u_i^y + \ell_i^y}{\mu} \right) - \mu \log |\mathcal{Y}|.
\]