
Structured Prediction via the Extragradient Method

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Abstract

We present a simple and scalable algorithm for large-margin estimation of structured models, including an important class of Markov networks and combinatorial models. We formulate the estimation problem as a convex-concave saddle-point problem and apply the extragradient method, yielding an algorithm with linear convergence using simple gradient and projection calculations. The projection step can be solved using combinatorial algorithms for min-cost quadratic flow. This makes the approach an efficient alternative to formulations based on reductions to a quadratic program (QP). We present experiments on two very different structured prediction tasks: 3D image segmentation and word alignment, illustrating the favorable scaling properties of our algorithm.

1 Introduction

The scope of discriminative learning methods has been expanding to encompass prediction tasks with increasingly complex structure. Much of this recent development builds upon graphical models to capture sequential, spatial, recursive or relational structure, but as we will discuss in this paper, the structured prediction problem is broader still. For graphical models, two major approaches to discriminative estimation have been explored: (1) maximum conditional likelihood [15] and (2) maximum margin [6, 1, 24]. For the broader class of models that we consider here, the conditional likelihood approach is intractable, but the large margin formulation yields tractable convex problems.

We interpret the term *structured output model* very broadly, as a compact scoring scheme over a (possibly very large) set of combinatorial structures and a method for finding the highest scoring structure. In graphical models, the scoring scheme is embodied in a probability distribution over possible assignments of the prediction variables as a function of input variables. In models based on combinatorial problems, the scoring scheme is usually a simple sum of weights associated with vertices, edges, or other components of a structure; these weights are often represented as parametric functions of a set of features. Given training instances labeled by desired structured outputs (e.g., matchings) and a set of

features that parameterize the scoring function, the learning problem is to find parameters such that the highest scoring outputs are as close as possible to the desired outputs.

Example of prediction tasks solved via combinatorial optimization problems include bipartite and non-bipartite matching in alignment of 2D shapes [5], word alignment in natural language translation [17] and disulfide connectivity prediction for proteins [3]. All of these problems can be formulated in terms of a tractable optimization problem. There are also interesting subfamilies of graphical models for which large-margin methods are tractable whereas likelihood-based methods are not; an example is the class of Markov random fields with restricted potentials used for object segmentation in vision [14, 2].

Tractability is not necessarily sufficient to obtain algorithms that work effectively in practice. In particular, although the problem of large margin estimation can be formulated as a quadratic program (QP) in several cases of interest [2, 23], and although this formulation exploits enough of the problem structure so as to achieve a polynomial representation in terms of the number of variables and constraints, off-the-shelf QP solvers scale poorly with problem and training sample size for these models. To solve large-scale machine learning problems, researchers often turn to simple gradient-based algorithms, in which each individual step is cheap in terms of computation and memory. Examples of this approach in the structured prediction setting include the Structured Sequential Minimal Optimization algorithm [24, 22] and the Structured Exponentiated Gradient algorithm [4]. These algorithms are first-order methods for solving QPs arising from low-treewidth Markov random fields and other decomposable models. They are able to scale to significantly larger problems than off-the-shelf QP solvers. However, they are limited in scope in that they rely on dynamic programming to compute essential quantities such as gradients. They do not extend to models in which dynamic programming is not applicable, for example, to problems such as matchings and min-cuts.

In this paper, we present an estimation methodology for structured prediction problems that does not require a general-purpose QP solver. We propose a saddle-point formulation which allows us to exploit simple gradient-based methods [13] with linear convergence guarantees. Moreover, we show that the key computational step in these methods—a certain projection operation—inherits the favorable computational complexity of the underlying optimization problem. This important result makes our approach viable computationally. In particular, for matchings and min-cuts, projection involves a min-cost quadratic flow computation, a problem for which efficient, highly-specialized algorithms are available. We illustrate the effectiveness of this approach on two very different large-scale structured prediction tasks: 3D image segmentation and word alignment in translation.

2 Structured models

We begin by discussing two special cases of the general framework that we subsequently present: (1) a class of Markov networks used for segmentation, and (2) a bipartite matching model for word alignment. Despite significant differences in the setup for these models, they share the property that in both cases the problem of finding the highest-scoring output can be formulated as a linear program (LP).

Markov networks. We consider a special class of Markov networks, common in vision applications, in which inference reduces to a tractable min-cut problem [8]. Focusing on binary variables, $\mathbf{y} = \{y_1, \dots, y_N\}$, and pairwise potentials, we define a joint distribution over $\{0, 1\}^N$ via $P(\mathbf{y}) \propto \prod_{j \in \mathcal{V}} \phi_j(y_j) \prod_{jk \in \mathcal{E}} \phi_{jk}(y_j, y_k)$, where $(\mathcal{V}, \mathcal{E})$ is an undirected graph, and where $\{\phi_j(y_j); j \in \mathcal{V}\}$ are the node potentials and $\{\phi_{jk}(y_j, y_k), jk \in \mathcal{E}\}$ are the edge potentials.

In image segmentation (see Fig. 1(a)), the node potentials capture local evidence about the label of a pixel or laser scan point. Edges usually connect nearby pixels in an image, and serve to correlate their labels. Assuming that such correlations tend to be *positive*

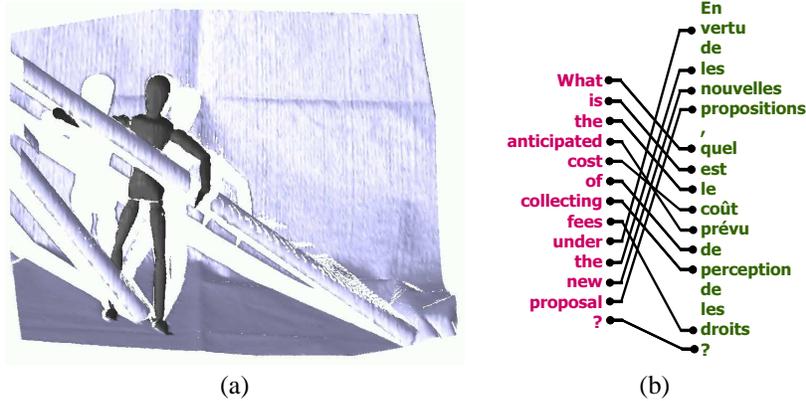


Figure 1: Examples of structured prediction applications: (a) articulated object segmentation and (b) word alignment in machine translation.

(connected nodes tend to have the same label), we restrict the form of edge potentials to be of the form $\phi_{jk}(y_j, y_k) = \exp\{-s_{jk} \mathbb{I}(y_j \neq y_k)\}$, where s_{jk} is a non-negative penalty for assigning y_j and y_k different labels. Expressing node potentials as $\phi_j(y_j) = \exp\{s_j y_j\}$, we have $P(\mathbf{y}) \propto \exp\left\{\sum_{j \in \mathcal{V}} s_j y_j - \sum_{jk \in \mathcal{E}} s_{jk} \mathbb{I}(y_j \neq y_k)\right\}$. Under this restriction of the potentials, it is known that the problem of computing the maximizing assignment, $\mathbf{y}^* = \arg \max P(\mathbf{y} \mid \mathbf{x})$, has a tractable formulation as a min-cut problem [8]. In particular, we obtain the following LP:

$$\max_{0 \leq z \leq 1} \sum_{j \in \mathcal{V}} s_j z_j - \sum_{jk \in \mathcal{E}} s_{jk} z_{jk} \quad \text{s.t.} \quad z_j - z_k \leq z_{jk}, \quad z_k - z_j \leq z_{jk}, \quad \forall jk \in \mathcal{E}. \quad (1)$$

In this LP, a continuous variable z_j is a relaxation of the binary variable y_j . Note that the constraints are equivalent to $|z_j - z_k| \leq z_{jk}$. Because s_{jk} is positive, $z_{jk} = |z_k - z_j|$ at the maximum, which is equivalent to $\mathbb{I}(z_j \neq z_k)$ if the z_j, z_k variables are binary. An integral optimal solution always exists, as the constraint matrix is totally unimodular [21] (that is, the relaxation is not an approximation).

We can parametrize the node and edge weights s_j and s_{jk} in terms of user-provided features \mathbf{x}_j and \mathbf{x}_{jk} associated with the nodes and edges. In particular, in 3D range data, \mathbf{x}_j might be spin image features or spatial occupancy histograms of a point j , while \mathbf{x}_{jk} might include the distance between points j and k , the dot-product of their normals, etc. The simplest model of dependence is a linear combination of features: $s_j = \mathbf{w}_n^\top \mathbf{f}_n(\mathbf{x}_j)$ and $s_{jk} = \mathbf{w}_e^\top \mathbf{f}_e(\mathbf{x}_{jk})$, where \mathbf{w}_n and \mathbf{w}_e are node and edge parameters, and \mathbf{f}_n and \mathbf{f}_e are node and edge feature mappings, of dimension d_n and d_e , respectively. To ensure non-negativity of s_{jk} , we assume the edge features \mathbf{f}_e to be non-negative and restrict $\mathbf{w}_e \geq 0$. This constraint is easily incorporated into the formulation we present below. We assume that the feature mappings \mathbf{f} are provided by the user and our goal is to estimate parameters \mathbf{w} from labeled data. We abbreviate the score assigned to a labeling \mathbf{y} for an input \mathbf{x} as $\mathbf{w}^\top \mathbf{f}(\mathbf{x}, \mathbf{y}) = \sum_j y_j \mathbf{w}_n^\top \mathbf{f}_n(\mathbf{x}_j) - \sum_{jk \in \mathcal{E}} y_{jk} \mathbf{w}_e^\top \mathbf{f}_e(\mathbf{x}_{jk})$, where $y_{jk} = \mathbb{I}(y_j \neq y_k)$.

Matchings. Consider modeling the task of word alignment of parallel bilingual sentences (see Fig. 1(b)) as a maximum weight bipartite matching problem, where the nodes $\mathcal{V} = \mathcal{V}^s \cup \mathcal{V}^t$ correspond to the words in the “source” sentence (\mathcal{V}^s) and the “target” sentence (\mathcal{V}^t) and the edges $\mathcal{E} = \{jk : j \in \mathcal{V}^s, k \in \mathcal{V}^t\}$ correspond to possible alignments between them. For simplicity, assume that each word aligns to one or zero words in the other sentence. The edge weight s_{jk} represents the degree to which word j in one sentence can translate into the word k in the other sentence. Our objective is to find an alignment that maximizes the sum of edge scores. We represent a matching using a set of binary variables

y_{jk} that are set to 1 if word j is assigned to word k in the other sentence, and 0 otherwise. The score of an assignment is the sum of edge scores: $s(\mathbf{y}) = \sum_{j,k \in \mathcal{E}} s_{jk} y_{jk}$. The maximum weight bipartite matching problem, $\arg \max_{\mathbf{y} \in \mathcal{Y}} s(\mathbf{y})$, can be found by solving the following LP:

$$\max_{0 \leq \mathbf{z} \leq 1} \sum_{j,k \in \mathcal{E}} s_{jk} z_{jk} \quad \text{s.t.} \quad \sum_{j \in \mathcal{V}^s} z_{jk} \leq 1, \forall k \in \mathcal{V}^t; \quad \sum_{k \in \mathcal{V}^t} z_{jk} \leq 1, \forall j \in \mathcal{V}^s, \quad (2)$$

where again the continuous variables z_{jk} correspond to the relaxation of the binary variables y_{jk} . As in the min-cut problem, this LP is guaranteed to have integral solutions for any scoring function $s(\mathbf{y})$ [21].

For word alignment, the scores s_{jk} can be defined in terms of the word pair jk and input features associated with \mathbf{x}_{jk} . We can include the identity of the two words, relative position in the respective sentences, part-of-speech tags, string similarity (for detecting cognates), etc. We let $s_{jk} = \mathbf{w}^\top \mathbf{f}(\mathbf{x}_{jk})$ for some user-provided feature mapping \mathbf{f} and abbreviate $\mathbf{w}^\top \mathbf{f}(\mathbf{x}, \mathbf{y}) = \sum_{j,k} y_{jk} \mathbf{w}^\top \mathbf{f}(\mathbf{x}_{jk})$.

General structure. More generally, we consider prediction problems in which the input $\mathbf{x} \in \mathcal{X}$ is an arbitrary structured object and the output is a vector of values $\mathbf{y} = (y_1, \dots, y_{L_x})$, for example, a matching or a cut in the graph. We assume that the length L_x and the structure of \mathbf{y} depend deterministically on the input \mathbf{x} . In our word alignment example, the output space is defined by the length of the two sentences. Denote the output space for a given input \mathbf{x} as $\mathcal{Y}(\mathbf{x})$ and the entire output space as $\mathcal{Y} = \bigcup_{\mathbf{x} \in \mathcal{X}} \mathcal{Y}(\mathbf{x})$.

Consider the class of structured prediction models \mathcal{H} defined by the linear family: $h_{\mathbf{w}}(\mathbf{x}) = \arg \max_{\mathbf{y} \in \mathcal{Y}(\mathbf{x})} \mathbf{w}^\top \mathbf{f}(\mathbf{x}, \mathbf{y})$, where $\mathbf{f}(\mathbf{x}, \mathbf{y})$ is a vector of functions $\mathbf{f} : \mathcal{X} \times \mathcal{Y} \mapsto \mathbb{R}^n$. This formulation is very general. Indeed, it is too general for our purposes—for many \mathbf{f}, \mathcal{Y} pairs, finding the optimal \mathbf{y} is intractable. Below, we specialize to the class of models in which the $\arg \max$ problem can be solved in polynomial time using linear programming (and more generally, convex optimization); this is still a very large class of models.

3 Max-margin estimation

We assume a set of training instances $S = \{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^m$, where each instance consists of a structured object \mathbf{x}_i (such as a graph) and a target solution \mathbf{y}_i (such as a matching). Consider learning the parameters \mathbf{w} in the conditional likelihood setting. We can define $P_{\mathbf{w}}(\mathbf{y} \mid \mathbf{x}) = \frac{1}{Z_{\mathbf{w}}(\mathbf{x})} \exp\{\mathbf{w}^\top \mathbf{f}(\mathbf{x}, \mathbf{y})\}$, where $Z_{\mathbf{w}}(\mathbf{x}) = \sum_{\mathbf{y}' \in \mathcal{Y}(\mathbf{x})} \exp\{\mathbf{w}^\top \mathbf{f}(\mathbf{x}, \mathbf{y}')\}$, and maximize the conditional log-likelihood $\sum_i \log P_{\mathbf{w}}(\mathbf{y}_i \mid \mathbf{x}_i)$, perhaps with additional regularization of the parameters \mathbf{w} . However, computing the partition function $Z_{\mathbf{w}}(\mathbf{x})$ is #P-complete [28, 11] for the two structured prediction problems we presented above, matchings and min-cuts. Instead, we adopt the max-margin formulation of [24], which directly seeks to find parameters \mathbf{w} such that: $\mathbf{y}_i = \arg \max_{\mathbf{y}'_i \in \mathcal{Y}_i} \mathbf{w}^\top \mathbf{f}(\mathbf{x}_i, \mathbf{y}'_i)$, $\forall i$, where $\mathcal{Y}_i = \mathcal{Y}(\mathbf{x}_i)$ and \mathbf{y}_i denotes the appropriate vector of variables for example i . The solution space \mathcal{Y}_i depends on the structured object \mathbf{x}_i ; for example, the space of possible matchings depends on the precise set of nodes and edges in the graph.

As in univariate prediction, we measure the error of prediction using a loss function $\ell(\mathbf{y}_i, \mathbf{y}'_i)$. To obtain a convex formulation, we upper bound the loss $\ell(\mathbf{y}_i, h_{\mathbf{w}}(\mathbf{x}_i))$ using the hinge function: $\max_{\mathbf{y}'_i \in \mathcal{Y}_i} [\mathbf{w}^\top \mathbf{f}_i(\mathbf{y}'_i) + \ell_i(\mathbf{y}'_i)] - \mathbf{w}^\top \mathbf{f}_i(\mathbf{y}_i)$, where $\ell_i(\mathbf{y}'_i) = \ell(\mathbf{y}_i, \mathbf{y}'_i)$, and $\mathbf{f}_i(\mathbf{y}'_i) = \mathbf{f}(\mathbf{x}_i, \mathbf{y}'_i)$. Minimizing this upper bound will force the true structure \mathbf{y}_i to be optimal with respect to \mathbf{w} for each instance i . We add a standard L_2 weight penalty $\frac{\|\mathbf{w}\|^2}{2C}$:

$$\min_{\mathbf{w} \in \mathcal{W}} \frac{\|\mathbf{w}\|^2}{2C} + \sum_i \max_{\mathbf{y}'_i \in \mathcal{Y}_i} [\mathbf{w}^\top \mathbf{f}_i(\mathbf{y}'_i) + \ell_i(\mathbf{y}'_i)] - \mathbf{w}^\top \mathbf{f}_i(\mathbf{y}_i), \quad (3)$$

where C is a regularization parameter and \mathcal{W} is the space of allowed weights (for example, $\mathcal{W} = \mathbb{R}^n$ or $\mathcal{W} = \mathbb{R}_+^n$). Note that this formulation is equivalent to the standard formulation using slack variables ξ and slack penalty C presented in [24, 23].

The key to solving Eq. (3) efficiently is the *loss-augmented inference problem*, $\max_{\mathbf{y}'_i \in \mathcal{Y}_i} [\mathbf{w}^\top \mathbf{f}_i(\mathbf{y}'_i) + \ell_i(\mathbf{y}'_i)]$. This optimization problem has precisely the same form as the prediction problem whose parameters we are trying to learn— $\max_{\mathbf{y}'_i \in \mathcal{Y}_i} \mathbf{w}^\top \mathbf{f}_i(\mathbf{y}'_i)$ —but with an additional term corresponding to the loss function. Tractability of the loss-augmented inference thus depends not only on the tractability of $\max_{\mathbf{y}'_i \in \mathcal{Y}_i} \mathbf{w}^\top \mathbf{f}_i(\mathbf{y}'_i)$, but also on the form of the loss term $\ell_i(\mathbf{y}'_i)$. A natural choice in this regard is the Hamming distance, which simply counts the number of variables in which a candidate solution \mathbf{y}'_i differs from the target output \mathbf{y}_i . In general, we need only assume that the loss function decomposes over the variables in \mathbf{y}_i .

For example, in the case of bipartite matchings the Hamming loss counts the number of different edges in the matchings \mathbf{y}_i and \mathbf{y}'_i and can be written as: $\ell_i^H(\mathbf{y}'_i) = \sum_{jk} y_{i,jk} + \sum_{jk} (1 - 2y'_{i,jk})y_{i,jk}$. Thus the loss-augmented matching problem for example i can be written as an LP similar to Eq. (2) (without the constant term $\sum_{jk} y_{i,jk}$):

$$\max_{0 \leq \mathbf{z} \leq 1} \sum_{jk} z_{i,jk} [\mathbf{w}^\top \mathbf{f}(\mathbf{x}_{i,jk}) + 1 - 2y_{i,jk}] \quad \text{s.t.} \quad \sum_j z_{i,jk} \leq 1, \quad \sum_k z_{i,jk} \leq 1.$$

Generally, when we can express $\max_{\mathbf{y}'_i \in \mathcal{Y}_i} \mathbf{w}^\top \mathbf{f}_i(\mathbf{y}'_i)$ as an LP, $\max_{\mathbf{z}_i \in \mathcal{Z}_i} \mathbf{w}^\top \mathbf{F}_i \mathbf{z}_i$, where $\mathcal{Z}_i = \{\mathbf{z}_i : \mathbf{A}_i \mathbf{z}_i \leq \mathbf{b}_i, \mathbf{z}_i \geq 0\}$, for appropriately defined constraints $\mathbf{A}_i, \mathbf{b}_i$ and feature matrix \mathbf{F}_i , we have a similar LP for the loss-augmented inference for each example i : $d_i + \max_{\mathbf{z}_i \in \mathcal{Z}_i} (\mathbf{w}^\top \mathbf{F}_i + \mathbf{c}_i)^\top \mathbf{z}_i$ for appropriately defined $d_i, \mathbf{F}_i, \mathbf{c}_i, \mathbf{A}_i, \mathbf{b}_i$. Let $\mathbf{z} = \{\mathbf{z}_1, \dots, \mathbf{z}_m\}$, $\mathcal{Z} = \mathcal{Z}_1 \times \dots \times \mathcal{Z}_m$.

We could proceed by making use of Lagrangian duality, which yields a joint convex optimization problem; this is the approach described in [23]. Instead we take a different tack here, posing the problem in its natural saddle-point form:

$$\min_{\mathbf{w} \in \mathcal{W}} \max_{\mathbf{z} \in \mathcal{Z}} \frac{\|\mathbf{w}\|^2}{2C} + \sum_i [\mathbf{w}^\top \mathbf{F}_i \mathbf{z}_i + \mathbf{c}_i^\top \mathbf{z}_i - \mathbf{w}^\top \mathbf{f}_i(\mathbf{y}_i)]. \quad (4)$$

As we discuss in the following section, this approach allows us to exploit the structure of \mathcal{W} and \mathcal{Z} *separately*, allowing for efficient solutions for a wider range of parameter and structure spaces.

4 Extragradient method

The key operations of the method we present below are gradient calculations and Euclidean projections. We let $L(\mathbf{w}, \mathbf{z}) = \frac{\|\mathbf{w}\|^2}{2C} + \sum_i [\mathbf{w}^\top \mathbf{F}_i \mathbf{z}_i + \mathbf{c}_i^\top \mathbf{z}_i - \mathbf{w}^\top \mathbf{f}_i(\mathbf{y}_i)]$, with gradients given by: $\nabla_{\mathbf{w}} L(\mathbf{w}, \mathbf{z}) = \frac{\mathbf{w}}{C} + \sum_i \mathbf{F}_i \mathbf{z}_i - \mathbf{f}_i(\mathbf{y}_i)$ and $\nabla_{\mathbf{z}_i} L(\mathbf{w}, \mathbf{z}) = \mathbf{F}_i^\top \mathbf{w} + \mathbf{c}_i$. We denote the projection of a vector \mathbf{z}_i onto \mathcal{Z}_i as $\pi_{\mathcal{Z}_i}(\mathbf{z}_i) = \arg \min_{\mathbf{z}'_i \in \mathcal{Z}_i} \|\mathbf{z}'_i - \mathbf{z}_i\|$ and similarly, the projection onto \mathcal{W} as $\pi_{\mathcal{W}}(\mathbf{w}') = \arg \min_{\mathbf{w} \in \mathcal{W}} \|\mathbf{w}' - \mathbf{w}\|$. A well-known solution strategy for saddle-point optimization is provided by the *extragradient method* [13]. An iteration of the extragradient method consists of two very simple steps, prediction $(\mathbf{w}, \mathbf{z}) \rightarrow (\mathbf{w}^p, \mathbf{z}^p)$ and correction $(\mathbf{w}^p, \mathbf{z}^p) \rightarrow (\mathbf{w}^c, \mathbf{z}^c)$:

$$\mathbf{w}^p = \pi_{\mathcal{W}}(\mathbf{w} - \beta \nabla_{\mathbf{w}} L(\mathbf{w}, \mathbf{z})); \quad \mathbf{z}_i^p = \pi_{\mathcal{Z}_i}(\mathbf{z}_i + \beta \nabla_{\mathbf{z}_i} L(\mathbf{w}, \mathbf{z})); \quad (5)$$

$$\mathbf{w}^c = \pi_{\mathcal{W}}(\mathbf{w} - \beta \nabla_{\mathbf{w}} L(\mathbf{w}^p, \mathbf{z}^p)); \quad \mathbf{z}_i^c = \pi_{\mathcal{Z}_i}(\mathbf{z}_i + \beta \nabla_{\mathbf{z}_i} L(\mathbf{w}^p, \mathbf{z}^p)); \quad (6)$$

where β is an appropriately chosen step size. The algorithm starts with a feasible point $\mathbf{w} = 0$, \mathbf{z}_i 's that correspond to the assignments \mathbf{y}_i 's and step size $\beta = 1$. After each prediction step, it computes $r = \beta \frac{\|\nabla L(\mathbf{w}, \mathbf{z}) - \nabla L(\mathbf{w}^p, \mathbf{z}^p)\|}{(\|\mathbf{w} - \mathbf{w}^p\| + \|\mathbf{z} - \mathbf{z}^p\|)}$. If r is greater than a threshold

ν , the step size is decreased using an Armijo type rule: $\beta = (2/3)\beta \min(1, 1/r)$, and a new prediction step is computed until $r \leq \nu$, where $\nu \in (0, 1)$ is a parameter of the algorithm. Once a suitable β is found, the correction step is taken and $(\mathbf{w}^c, \mathbf{z}^c)$ becomes the new (\mathbf{w}, \mathbf{z}) . The method is guaranteed to converge linearly to a solution $\mathbf{w}^*, \mathbf{z}^*$ [13, 10]. See Appendix A for details. By comparison, Exponentiated Gradient [4] has sublinear convergence rate guarantees, while Structured SMO [22] has none.

The key step influencing the efficiency of the algorithm is the Euclidean projection onto the feasible sets \mathcal{W} and \mathcal{Z}_i . In case $\mathcal{W} = \mathbb{R}^n$, the projection is the identity operation; projecting onto \mathbb{R}_+^n consists of clipping negative weights to zero. Additional problem-specific constraints on the weight space can be efficiently incorporated in this step (although linear convergence guarantees only hold for polyhedral \mathcal{W}). In case of word alignment, \mathcal{Z}_i is the convex hull of bipartite matchings and the problem reduces to the much-studied minimum cost quadratic flow problem. The projection $\mathbf{z}_i = \pi_{\mathcal{Z}_i}(\mathbf{z}'_i)$ is given by

$$\min_{0 \leq z \leq 1} \sum_{jk} \frac{1}{2} (z'_{i,jk} - z_{i,jk})^2 \quad \text{s.t.} \quad \sum_j z_{i,jk} \leq 1, \quad \sum_k z_{i,jk} \leq 1.$$

We use a standard reduction of bipartite matching to min-cost flow by introducing a source node s linked to all the nodes in \mathcal{V}_i^s (words in the “source” sentence), and a sink node t linked from all the nodes in \mathcal{V}_i^t (words in the “target” sentence), using edges of capacity 1 and cost 0. The original edges jk have a quadratic cost $\frac{1}{2}(z'_{i,jk} - z_{i,jk})^2$ and capacity 1. Minimum (quadratic) cost flow from s to t is the projection of \mathbf{z}'_i onto \mathcal{Z}_i .

The reduction of the projection to minimum quadratic cost flow for the min-cut polytope \mathcal{Z}_i is shown in Appendix B. Algorithms for solving this problem are nearly as efficient as those for solving regular min-cost flow problems. In case of word alignment, the running time scales with the cube of the sentence length. We use publicly-available code for solving this problem [9] (see http://www.math.washington.edu/~tseng/netflowg_nl/).

5 Experiments

We investigate two structured models we described above: bipartite matchings for word alignments and restricted potential Markov nets for 3D segmentation. A commercial QP-solver, MOSEK, runs out of memory on the problems we describe below using the QP formulation [23]. We compared the extragradient method with the averaged perceptron algorithm [6]. A question which arises in practice is how to choose the regularization parameter C . The typical approach is to run the algorithm for several values of the regularization parameter and pick the best model using a validation set. For the averaged perceptron, a standard method is to run the algorithm tracking its performance on a validation set, and selecting the model with best performance. We use the same training regime for the extragradient by running it with $C = \infty$.

Object segmentation. We test our algorithm on a 3D scan segmentation problem using the class of Markov networks with potentials that were described above. The dataset is a challenging collection of cluttered scenes containing articulated wooden puppets [2]. It contains eleven different single-view scans of three puppets of varying sizes and positions, with clutter and occluding objects such as rope, sticks and rings. Each scan consists of around 7,000 points. Our goal was to segment the scenes into two classes—puppet and background. We use five of the scenes for our training data, three for validation and three for testing. Sample scans from the training and test set can be seen at <http://www.cs.berkeley.edu/~taskar/3Dsegment/>. We computed spin images of size 10×5 bins at two different resolutions, then scaled the values and performed PCA to obtain 45 principal components, which comprised our node features. We used the surface links output by the scanner as edges between points and for each edge only used a single feature, set to a constant value of 1 for all edges. This results in all edges having the same potential. The training data contains approximately 37,000 nodes and 88,000 edges.

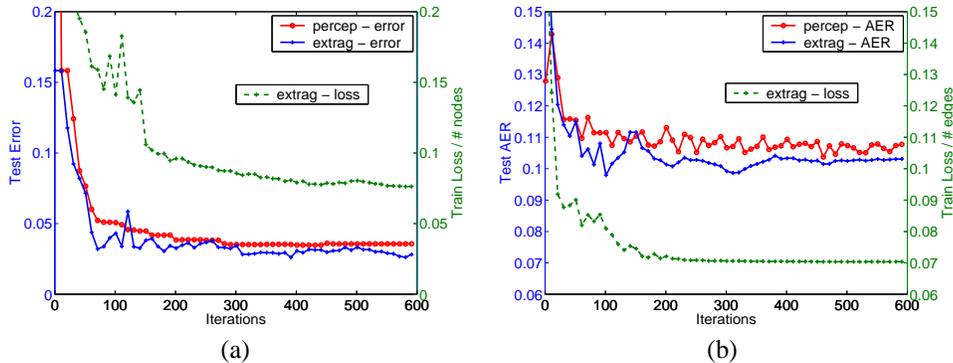


Figure 2: Both plots show test error for the averaged perceptron and the extragradient (left y-axis) and training loss per node or edge for the extragradient (right y-axis) versus number of iterations for (a) object segmentation task and (b) word alignment task.

Training time took about 4 hours for 600 iterations on a 2.80GHz Pentium 4 machine. Fig. 2(a) shows that the extragradient has a consistently lower error rate (about 3% for extragradient, 4% for averaged perceptron), using only slightly more expensive computations per iteration. Also shown is the corresponding decrease in the hinge-loss upperbound on the training data as the extragradient progresses.

Word alignment. We also tested our learning algorithm on word-level alignment using a data set from the 2003 NAACL set [18], the English-French Hansards task. This corpus consists of 1.1M automatically aligned sentences, and comes with a validation set of 39 sentence pairs and a test set of 447 sentences. The validation and test sentences have been hand-aligned and are marked with both *sure* and *possible* alignments. Using these alignments, *alignment error rate* (AER) is calculated as: $AER(A, S, P) = 1 - \frac{|A \cap S| + |A \cap P|}{|A| + |S|}$. Here, A is a set of proposed index pairs, S is the set of sure gold pairs, and P is the set of possible gold pairs (where $S \subseteq P$).

We used the intersection of the predictions of the English-to-French and French-to-English IBM Model 4 alignments (using GIZA++ [19]) on the first 5000 sentence pairs from the 1.1M sentences. The number of edges for 5000 sentences was about 555,000. We tested on the 347 hand-aligned test examples, and used the validation set to select the stopping point. The features on the word pair (e_j, f_k) include measures of association, orthography, relative position, predictions of generative models (see [26] for details). It took about 3 hours to perform 600 training iterations on the training data using a 2.8GHz Pentium 4 machine. Fig. 2(b) shows the extragradient performing slightly better (by about 0.5%) than average perceptron.

6 Conclusion

We have presented a general solution strategy for large-scale structured prediction problems. We have shown that these problems can be formulated as saddle-point optimization problems, problems that are amenable to solution by the extragradient algorithm. Key to our approach is the recognition that the projection step in the extragradient algorithm can be solved by network flow algorithms. Network flow algorithms are among the most well-developed in the field of combinatorial optimization, and yield stable, efficient algorithmic platforms. We have exhibited the favorable scaling of this overall approach in two concrete, large-scale learning problems. It is also important to note that the general approach extends to a much broader class of problems. In [25], we show how to apply this approach efficiently to other types of models, including general Markov networks and weighted context-free grammars, using Bregman projections.

Acknowledgments

We thank Paul Tseng for kindly answering our questions about his min-cost flow code. This work was funded by the DARPA CALO project (03-000219) and Microsoft Research MICRO award (05-081). SLJ was also supported by an NSERC graduate scholarship.

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A Convergence analysis

The convergence analysis of the extragradient method is based on a more general framework of variational inequalities [7]. We begin by establishing some notation and definitions. Because the optimization is over a convex set, a feasible point $(\mathbf{w}^*, \mathbf{z}^*)$, with $\mathbf{w}^* \in \mathcal{W}, \mathbf{z}^* \in \mathcal{Z}$, is a solution of Eq. (4) if and only if

$$\begin{aligned} \nabla_{\mathbf{w}} L(\mathbf{w}^*, \mathbf{z}^*)^\top (\mathbf{w} - \mathbf{w}^*) &\geq 0, & \forall \mathbf{w} \in \mathcal{W}; \\ \nabla_{\mathbf{z}_i} L(\mathbf{w}^*, \mathbf{z}^*)^\top (\mathbf{z}_i - \mathbf{z}_i^*) &\leq 0, & \forall i, \forall \mathbf{z}_i \in \mathcal{Z}_i. \end{aligned}$$

Let us combine \mathbf{w} and \mathbf{z} into one vector:

$$\mathbf{u} = \begin{pmatrix} \mathbf{w} \\ \mathbf{z}_1 \\ \vdots \\ \mathbf{z}_m \end{pmatrix}; \quad \mathcal{U} = \left\{ \begin{pmatrix} \mathbf{w} \\ \mathbf{z}_1 \\ \vdots \\ \mathbf{z}_m \end{pmatrix} : \mathbf{w} \in \mathcal{W}, \mathbf{z}_i \in \mathcal{Z}_i, \forall i \right\},$$

and denote the projection operator onto \mathcal{U} as $\pi_{\mathcal{U}}(\mathbf{v}) = \arg \min_{\mathbf{u} \in \mathcal{U}} \|\mathbf{u} - \mathbf{v}\|$. Note that \mathcal{U} is convex since it is a direct product of convex sets. We denote the (affine) gradient operator on this joint space as

$$T(\mathbf{u}) = \begin{pmatrix} \nabla_{\mathbf{w}} L(\mathbf{w}, \mathbf{z}) \\ -\nabla_{\mathbf{z}_1} L(\mathbf{w}, \mathbf{z}) \\ \vdots \\ -\nabla_{\mathbf{z}_m} L(\mathbf{w}, \mathbf{z}) \end{pmatrix} = \begin{pmatrix} \mathbf{I}/C \mathbf{F}_1 \cdots \mathbf{F}_m \\ -\mathbf{F}_1^\top \\ \vdots \\ 0 \\ -\mathbf{F}_m^\top \end{pmatrix} \begin{pmatrix} \mathbf{w} \\ \mathbf{z}_1 \\ \vdots \\ \mathbf{z}_m \end{pmatrix} - \begin{pmatrix} \sum \mathbf{f}_i(\mathbf{y}_i) \\ \mathbf{c}_1 \\ \vdots \\ \mathbf{c}_m \end{pmatrix} = \mathbf{F}\mathbf{u} - \mathbf{a},$$

where \mathbf{I} in the upper-left corner of the \mathbf{F} is the identity matrix of appropriate size.

With these definitions, the optimality condition for a point $\mathbf{u}^* \in \mathcal{U}$ becomes:

$$T(\mathbf{u}^*)^\top (\mathbf{u}' - \mathbf{u}^*) \geq 0, \quad \forall \mathbf{u}' \in \mathcal{U}. \quad (7)$$

We denote the set of solutions satisfying these conditions as \mathcal{U}^* . Problems of this form are called variational inequalities and arise in many important applications such as optimization, solving system of equations and market equilibrium [7].

Let us define a residual error function for Eq. (7):

$$e(\mathbf{u}, \beta) = \mathbf{u} - \pi_{\mathcal{U}}(\mathbf{u} - \beta T(\mathbf{u})).$$

Note that for $\beta > 0$, the zeros of $e(\mathbf{u}, \beta)$ are precisely the solutions of Eq. (7):

$$e(\mathbf{u}, \beta) = 0 \quad \Leftrightarrow \quad \mathbf{u} \in \mathcal{U}^*. \quad (8)$$

This is a consequence of a characterization of the projection of an arbitrary point \mathbf{v} onto a convex set \mathcal{U} ; let $\mathbf{u} \in \mathcal{U}$, then we have:

$$(\mathbf{v} - \mathbf{u})^\top (\mathbf{u}' - \mathbf{u}) \leq 0, \quad \forall \mathbf{u}' \in \mathcal{U} \quad \Leftrightarrow \quad \mathbf{u} = \pi_{\mathcal{U}}(\mathbf{v}). \quad (9)$$

Assume $e(\mathbf{u}, \beta) = 0$, $\beta > 0$ and let $\mathbf{v} = \mathbf{u} - \beta T(\mathbf{u})$. Since $e(\mathbf{u}, \beta) = 0$, $\mathbf{u} = \pi_{\mathcal{U}}(\mathbf{v}) = \pi_{\mathcal{U}}(\mathbf{u} - \beta T(\mathbf{u}))$. Plugging \mathbf{v} in Eq. (9), shows that \mathbf{u} satisfies the optimality condition in Eq. (7). Conversely, assume \mathbf{u}^* satisfies Eq. (7) and let $\mathbf{u}^+ = \pi_{\mathcal{U}}(\mathbf{u}^* - \beta T(\mathbf{u}^*))$. By Eq. (9), we have

$$(\mathbf{u}^* - \beta T(\mathbf{u}^*) - \mathbf{u}^+)^\top (\mathbf{u}' - \mathbf{u}^+) = (\mathbf{u}^* - \mathbf{u}^+)^\top (\mathbf{u}' - \mathbf{u}^+) - \beta T(\mathbf{u}^*)^\top (\mathbf{u}' - \mathbf{u}^+) \leq 0, \quad \forall \mathbf{u}' \in \mathcal{U}.$$

In particular, for $\mathbf{u}' = \mathbf{u}^*$, we have $\|\mathbf{u}^* - \mathbf{u}^+\|^2 \leq \beta T(\mathbf{u}^*)^\top (\mathbf{u}^* - \mathbf{u}^+)$. Since the right-hand-side, $\beta T(\mathbf{u}^*)^\top (\mathbf{u}^* - \mathbf{u}^+)$, is non-positive by Eq. (7), and the left-hand-side is non-negative, we have $\mathbf{u} = \mathbf{u}^+$ and hence $e(\mathbf{u}, \beta) = 0$.

We will make use of the following theorem (which holds for more general operators $T(\mathbf{u})$) to prove the convergence of the extragradient method for structured prediction problems.

Theorem A.1 (Theorem 2.1 in [10]) *Let $\{\beta_k\}$ be a sequence such that $\inf_k \{\beta_k\} = \beta_{\min} > 0$ and let $c_0 > 0$ be a constant. If the sequence $\{\mathbf{u}^k\}$ satisfies:*

$$\|\mathbf{u}^{k+1} - \mathbf{u}^*\|^2 \leq \|\mathbf{u}^k - \mathbf{u}^*\|^2 - c_0 \|e(\mathbf{u}^k, \beta_k)\|^2, \quad \forall \mathbf{u}^* \in \mathcal{U}^*, \quad (10)$$

then $\{\mathbf{u}^k\}$ converges to a solution point of Eq. (7).

The extragradient algorithm can be written as:

$$\begin{aligned} (P) \quad \bar{\mathbf{u}}^{k+1} &= \pi_{\mathcal{U}}(\mathbf{u}^k - \beta_k T(\mathbf{u}^k)); \\ (C) \quad \mathbf{u}^{k+1} &= \pi_{\mathcal{U}}(\mathbf{u}^k - \beta_k T(\bar{\mathbf{u}}^{k+1})), \end{aligned}$$

with $r_k = \beta_k \|T(\mathbf{u}^k) - T(\bar{\mathbf{u}}^{k+1})\| / \|\mathbf{u}^k - \bar{\mathbf{u}}^{k+1}\|$. Under the assumption that $r_k < \nu < 1$, Korpelevich [13] showed that for the extragradient, $c_0 = (1 - \nu)^2$ in Eq. (10):

$$\|\mathbf{u}^{k+1} - \mathbf{u}^*\|^2 \leq \|\mathbf{u}^k - \mathbf{u}^*\|^2 - (1 - \nu)^2 \|e(\mathbf{u}^k, \beta_k)\|^2, \quad \forall \mathbf{u}^* \in \mathcal{U}^*,$$

It remains to show that we can lower bound β_k away from zero for the Armijo type rule $\beta_k = (2/3)\beta_k \min(1, 1/r_k)$. Note that

$$\max_{\mathbf{u}, \mathbf{v}} \frac{\|T(\mathbf{u}) - T(\mathbf{v})\|}{\|\mathbf{u} - \mathbf{v}\|} = \max_{\|\mathbf{u}\|=1} \|\mathbf{F}\mathbf{u}\| = \|\mathbf{F}\|,$$

where $\|\mathbf{F}\|$ is the standard matrix norm induced by the Euclidean vector norm $\|\cdot\|$. Hence, $\beta_k < \nu / \|\mathbf{F}\|$ ensures $r_k < \nu$, which leaves β_k constant and away from zero. The norm of \mathbf{F} ultimately depends on the problem (mincut or matching), the number of examples and the feature map $\mathbf{f}(\mathbf{x}, \mathbf{y})$.

The local linear convergence of the extragradient method is well established for affine $T(\mathbf{u})$ and polyhedral \mathcal{U} [16, 27]. Let $d(\mathbf{u}, \mathcal{U}^*)$ be the shortest distance from \mathbf{u} to a solution of Eq. (7): $d(\mathbf{u}, \mathcal{U}^*) = \inf_{\mathbf{u}^* \in \mathcal{U}^*} \|\mathbf{u} - \mathbf{u}^*\|$. Note that Eq. (10) implies that

$$d(\mathbf{u}^{k+1}, \mathcal{U}^*)^2 \leq d(\mathbf{u}^k, \mathcal{U}^*)^2 - c_0 \|e(\mathbf{u}^k, \beta_k)\|^2. \quad (11)$$

To prove local linear convergence, it suffices to show that for some constants $\epsilon > 0, c_1 > 0$,

$$d(\mathbf{u}, \mathcal{U}^*) \leq c_1 \|e(\mathbf{u}, \beta_k)\|, \quad \forall \mathbf{u} \in \mathcal{U}, \quad \text{whenever} \quad \|e(\mathbf{u}, \beta_k)\| \leq \epsilon,$$

which implies that for sufficiently large k ,

$$\frac{d(\mathbf{u}^{k+1}, \mathcal{U}^*)}{d(\mathbf{u}^k, \mathcal{U}^*)} \leq \sqrt{1 - \frac{c_0}{c_1^2}} \quad (12)$$

For polyhedral spaces $\mathcal{U} = \{\mathbf{u} : \mathbf{u} \geq 0; \mathbf{A}\mathbf{u} \leq \mathbf{b}\}$, the constant is given by

$$c_1 = \|\mathbf{A}^\top\| / \lambda(\mathbf{B}\mathbf{B}^\top),$$

where $\lambda(\mathbf{B}\mathbf{B}^\top)$ is the smallest eigenvalue of the matrix $\mathbf{B}\mathbf{B}^\top$, with \mathbf{B} formed by linearly independent rows of \mathbf{A} corresponding to constraints active at the solution [20, 16].

B Min-cut polytope projections

Consider projection for a single example i :

$$\begin{aligned} \min_{\mathbf{z}} \quad & \sum_{j \in \mathcal{V}} \frac{1}{2} (z'_j - z_j)^2 + \sum_{jk \in \mathcal{E}} \frac{1}{2} (z'_{jk} - z_{jk})^2 \\ \text{s.t.} \quad & 0 \leq z_j \leq 1, \quad \forall j; \quad z_j - z_k \leq z_{jk}, \quad z_k - z_j \leq z_{jk}, \quad \forall jk. \end{aligned} \quad (13)$$

Let $h_j^+(z_j) = \frac{1}{2}(z'_j - z_j)^2$ if $0 \leq z_j$, else ∞ . We introduce non-negative Lagrangian variables $\lambda_{jk}, \lambda_{kj}$ for the two constraints for each edge jk and λ_{j0} for the constraint $z_j \leq 1$ each node j .

The Lagrangian is given by:

$$\begin{aligned} L(\mathbf{z}, \lambda) = & \sum_j h_j^+(z_j) + \sum_{jk} \frac{1}{2} (z'_{jk} - z_{jk})^2 - \sum_j (1 - z_j) \lambda_{j0} \\ & - \sum_{jk} (z_{jk} - z_j + z_k) \lambda_{jk} - \sum_{jk} (z_{jk} - z_k + z_j) \lambda_{kj} \end{aligned}$$

Letting $\lambda_{0j} = \lambda_{j0} + \sum_{k:jk \in \mathcal{E}} (\lambda_{jk} - \lambda_{kj})$, note that

$$\sum_j z_j \lambda_{0j} = \sum_j z_j \lambda_{j0} + \sum_{jk} (z_j - z_k) \lambda_{jk} + \sum_{jk} (z_k - z_j) \lambda_{kj}.$$

So the Lagrangian becomes:

$$L(\mathbf{z}, \lambda) = \sum_j h_j^+(z_j) + z_j \lambda_{0j} - \lambda_{j0} + \sum_{jk} \frac{1}{2} (z'_{jk} - z_{jk})^2 - z_{jk} (\lambda_{jk} + \lambda_{kj}).$$

Now, minimizing $L(\mathbf{z}, \lambda)$ with respect to \mathbf{z} , we have

$$\inf_{\mathbf{z}} L(\mathbf{z}, \lambda) = \sum_{jk} q_{jk} (\lambda_{jk} + \lambda_{kj}) + \sum_j q_{0j} (\lambda_{0j}) - \lambda_{j0},$$

where $q_{jk} (\lambda_{jk} + \lambda_{kj}) = \inf_{z_{jk}} \left[\frac{1}{2} (z'_{jk} - z_{jk})^2 - z_{jk} (\lambda_{jk} + \lambda_{kj}) \right]$ and $q_{0j} (\lambda_{0j}) = \inf_{z_j} [h_j^+(z_j) + z_j \lambda_{0j}]$. The minimizing values of \mathbf{z} are:

$$\begin{aligned} z_j^* &= \arg \inf_{z_j} [h_j^+(z_j) + z_j \lambda_{0j}] = \begin{cases} 0 & \lambda_{0j} \geq z'_j; \\ z'_j - \lambda_{0j} & \lambda_{0j} \leq z'_j; \end{cases} \\ z_{jk}^* &= \arg \inf_{z_{jk}} \left[\frac{1}{2} (z'_{jk} - z_{jk})^2 - z_{jk} (\lambda_{jk} + \lambda_{kj}) \right] = z'_{jk} + \lambda_{jk} + \lambda_{kj}. \end{aligned}$$

Hence, we have:

$$\begin{aligned}
q_{jk}(\lambda_{jk} + \lambda_{kj}) &= -z'_{jk}(\lambda_{jk} + \lambda_{kj}) - \frac{1}{2}(\lambda_{jk} + \lambda_{kj})^2 \\
q_{0j}(\lambda_{0j}) &= \begin{cases} \frac{1}{2}z_j'^2 & \lambda_{0j} \geq z_j' \\ z_j'\lambda_{0j} - \frac{1}{2}\lambda_{0j}^2 & \lambda_{0j} \leq z_j' \end{cases}
\end{aligned}$$

The dual of the projection problem is thus:

$$\begin{aligned}
\max_{\lambda} \quad & \sum_j q_{0j}(\lambda_{0j}) - \lambda_{j0} + \sum_{jk} -z'_{jk}(\lambda_{jk} + \lambda_{kj}) - \frac{1}{2}(\lambda_{jk} + \lambda_{kj})^2 \quad (14) \\
\text{s.t.} \quad & \lambda_{j0} - \lambda_{0j} + \sum_{jk} (\lambda_{jk} - \lambda_{kj}) = 0, \quad \forall j; \\
& \lambda_{jk}, \lambda_{kj} \geq 0, \quad \forall jk; \quad \lambda_{j0} \geq 0, \quad \forall j.
\end{aligned}$$

Interpreting λ_{jk} as flow from node j to node k , and λ_{kj} as flow from k to j and $\lambda_{j0}, \lambda_{0j}$ as flow from and to a special node 0, we can identify the constraints of Eq. (14) as conservation of flow constraints. The last transformation we need is to address the presence of cross-terms $\lambda_{jk}\lambda_{kj}$ in the objective. Note that in the flow conservation constraints, $\lambda_{jk}, \lambda_{kj}$ always appear together as $\lambda_{jk} - \lambda_{kj}$. Since we are minimizing $(\lambda_{jk} + \lambda_{kj})^2$ subject to constraints on $\lambda_{jk} - \lambda_{kj}$, at least one of $\lambda_{jk}, \lambda_{kj}$ will be zero at the optimum and the cross-terms can be ignored. Note that all λ variables are non-negative except for λ_{0j} 's. Many standard flow packages support this problem form, but we can also transform the problem to have all non-negative flows by introducing extra variables. The final form has a convex cost for each edge:

$$\begin{aligned}
\min_{\lambda} \quad & \sum_j -q_{0j}(\lambda_{0j}) + \lambda_{j0} + \sum_{jk} z'_{jk}\lambda_{jk} + \frac{1}{2}\lambda_{jk}^2 + \sum_{jk} z'_{jk}\lambda_{kj} + \frac{1}{2}\lambda_{kj}^2 \quad (15) \\
\text{s.t.} \quad & \lambda_{j0} - \lambda_{0j} + \sum_{jk} \lambda_{jk} - \lambda_{kj} = 0, \quad \forall j; \\
& \lambda_{jk}, \lambda_{kj} \geq 0, \quad \forall jk; \quad \lambda_{j0} \geq 0, \quad \forall j.
\end{aligned}$$