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A dual method for solving the nonlinear structured prediction problem☆

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ABSTRACT

In this paper, we present a perceptron-based algorithm and have developed a dual formulation to solve the nonlinear structured prediction problem, which we called Dual Structured Incremental Margin Algorithm (DSIMA). The proposed formulation allows the introduction of kernel functions enabling the efficient solution of nonlinear problems. In order to verify the correctness and applicability of the algorithm, we consider an inverse approach to the path planning problem. The problem mapped on a grid environment can be solved by a search process that essentially depends on the definition of the transition costs between states. In this context, we develop and apply a learning algorithm that is able to perform the reverse path, i.e., the prediction of these costs in a direct space for the linear form. However, considering the nonlinear form, the problem is solved in a space of high dimension and where it is possible to learn a path instead of the transition costs. This learning problem is usually formulated as a convex optimization problem of maximum margin. Several tests to solve the costs prediction problem were carried out and the results compared to other structured prediction techniques. The proposed algorithm demonstrated greater efficiency in terms of computational effort and quality of prediction.

1. Introduction

One of the fundamental problems in learning theory is the construction of classifiers that are capable of efficient generalization performance. Meanwhile, structured learning has recently gained attention within the machine learning community as a tractable method of solving several learning problems, e.g., the detection and classification of objects for video scenes [13], for learning a policy from demonstration [6] or for learning the transition costs in the inverse path planning problem [8].

However, because of scalability, current methods are limited in terms of memory requirement in the dual space with an explosive number of variables and in the primal space, with the dependence on the domain. Therefore, the main objective of this paper is to present the development of the DSIMA, demonstrating its applicability and efficiency in relation to their respective examples and without the mentioned limitations.

The structured prediction problem is formulated as a convex optimization problem of maximum margin and its structure is very similar to the formulation of multi-class support vector machines [16]. As a solution method, we proposed previously in Coelho et al. [2] a relaxation procedure based on a primal formulation of the perceptron model, called Structured Incremental Margin Algorithm, efficient at solving linearly separable problems. However, if we use a linear algorithm to solve a nonlinearly separable classification problem, we cannot obtain a linear hypothesis that produces the correct separation of two classes in the input space. Also, in nonlinear structured prediction problems, we cannot obtain a hyperplane where the computed distance in relation to the expert's choices is greater than or equal to the computed distance of any other choice. In both cases, this results in obtaining negative margins.

There are two common approaches to deal with nonlinearity. The first, proposed by Taskar [11], consists in obtaining the dual of the maximum margin structured prediction problem with the use of kernel functions. To solve this problem the author uses an adaptation of the Sequential Minimal Optimization (SMO) method [7]. The formulation leads to the solution of a quadratic programming problem with a large number of variables in the dual space. The second, proposed by Ratliff et al. [9], considers the primal formulation of the problem and adopts an expanded set of features that increases the size of the direct space. This solution employs a technique known as Structured Boosting [5]. In that work, the authors developed the MMPBoost algorithm, which is applied to solve a nonlinear inverse path planning problem. This construction technique promotes an *ad hoc* solution, being dependent on the

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application domain. Our proposal, the DSIMA, avoids an excessive number of variables as well as the dependence on the application domain.

The inverse path planning problem was also used to test the proposed algorithm. The design or layout of paths is only possible from the prior knowledge of the cost matrix, which reflects the transition costs. The approach presented provides a solution to the inverse problem: the discovery of the cost matrix from a set of samples planned by an expert. In these problems, the major difficulty is the definition of costs in a precise way for different types of terrains on the maps reflecting the choice of a set of features. These costs need to be known and reliable. This paper indicates how to predict these costs and new paths in nonlinear problems. In this case, only a nonlinear function of the set of features could provide a learning strategy.

The problem discussed here has a direct relationship with inverse reinforcement learning, proposed by Russell [10]. In both problems, the goal is to learn a policy or trajectory defined by a reward function associated with the execution of a task using a set of observations defined by an expert. The basic principle is to guarantee that the expert acts optimally for an unknown reward function. This is the opposite of the direct problem of reinforcement learning, where the reward function or immediate return of the actions is known and the goal is the definition of a maximization policy of the cumulative returns.

In the linear case, we can learn the cost values that subsequently allow the definition of an optimal policy in new scenarios with the aid of an optimization algorithm. But, in the nonlinear case, we are able to predict only complete new paths in accordance with the expert strategy. This is due to the use of kernel functions. Also, unlike what occurs in the inverse reinforcement learning problem, where the direct reinforcement learning problem is repeatedly solved, this inference process is based only on the observation of the samples given. The work of Klein et al. [4] presents a similar approach for solving the inverse problem of reinforcement learning associated with structured classification. The paper reflects with more accuracy the maximization of the margin between the best policy obtained within an updated estimate and the policy implemented by the expert.

In order to evaluate the efficiency of the proposed algorithm, linear and nonlinear examples were used. The obtained results were compared with the Maximum Margin Planning (MMP) [8] and MMPBoost [9], techniques according to the expectations, always demonstrating a strong association between the output obtained by the algorithm and the planning of new paths following the expert's strategy. Applied to the inverse path planning problem this learning strategy permits us to obtain plans from the perception of the features of maps. This information is of great importance to be used in any path planning applications, such as the layout of roads and railways, paths for robots and autonomous vehicles.

The remainder of this paper is organized as follows. Section 2 describes preliminary concepts concerned with the structured prediction model and the solution for the linear case based on a primal formulation of the structured perceptron. Section 3 addresses the nonlinear case and the dual formulation proposed for the structured perceptron, including the kernel functions. Section 4 reports the costs prediction problem. In Section 5 we describe the experiments and present the obtained results. Finally, in Section 6, some considerations and conclusions about the work are reported.

2. Structured prediction model

Given a training set $S = \{(x_i, y_i),\ i = 1, \dots, m\}$, each pair is formed by a sample represented by a structured object x_i and a desirable solution y_i. The function f describes an association between the input x_i and an output y which is usually defined by a linear operator, resulting in a vector $f(x_i, y)$ called feature vector. The goal is to obtain a parameter vector w such that:

$$\arg\min_{y \in Y_i} \left\{ w^T f(x_i, y) \right\} \approx y, i = 1, \dots, m, \tag{1}$$

where Y_i is the set of all possible solutions related to the structured object x_i. The cardinality of Y_i can be very high, but we can use techniques that efficiently choose the best candidates y. Hence, learning the parameter vector w allows us to reach the best solution for each pair (x_i, y) that is exactly the solution $y_i \in S$.

2.1. Maximum margin approach

The approach to solve this problem is based on a generalization of the principle of maximum margin [12] used in support vector machines [15] and requires the solution of the following quadratic programming problem related to the minimization of the vector norm:

$$\begin{aligned} &\min 1/2\, w_2^2 \\ &\text{subject to :} \\ &w^T f(x_i, y) - w^T f(x_i, y_i) \geq l_i(y),\ \ \forall i, \forall y \in Y_i, \end{aligned} \tag{2}$$

where the function $l_i(y)$ is defined as a loss function that scales the geometric value of the margin. Introducing the optimization process, which allows us to choose the best candidate, we can express the problem in the form:

$$\begin{aligned} &\min 1/2\, w_2^2 \\ &\text{subject to :} \\ &w^T f(x_i, y_i) \leq \min_{y \in Y(i)} \left\{ w^T f(x_i, y) - l_i(y) \right\},\ \ i = 1, \dots, m. \end{aligned} \tag{3}$$

The margin γ_i of a sample (x_i, y_i) compared to another element $y \in Y_i$ is interpreted as:

$$\gamma_{y_i, y} = \left(w^T f(x_i, y) - w^T f(x_i, y_i) \right) / w_2. \tag{4}$$

When we compare this element to all the other elements $y \in Y_i$ and $y \neq y_i$, the margin of each sample is given by:

$$\gamma_i = \left(\min_{y \in Y_i,\ y \neq y_i} \left\{ w^T f(x_i, y) - w^T f(x_i, y_i) \right\} \right) / w_2. \tag{5}$$

The final margin will be considered as the minimum value of all margins, i.e., $\gamma = \min\{y_i\},\ \ i = 1,\ \dots,\ m.$

Tsochantaridis et al. [14] consider a margin parameter that must be maximized with an additional restriction: the control of the w norm. So, the problem (3) can be rewritten as:

$$\begin{aligned} &\max \gamma \\ &\text{subject to :} \\ &\min_{y \in Y_i} \left\{ w^T f(x_i, y) - l_i(y) \right\} - w^T f(x_i, y_i) \geq \gamma, i = 1, \dots, m. \end{aligned} \tag{6}$$

Consequently, minimizing the Euclidean norm of vector w or, equivalently, maximizing the margin γ, results in obtaining a solution of maximum margin. For cases with nonlinearity we can introduce slack variables or use a dual formulation with the introduction of kernel functions. Note that the optimization problem $\min_{y \in Y_i} \{w^T f(x_i, y) - l_i(y)\}$ is similar to the original problem associated with structured learning. In general, this problem has polynomial complexity, such as a shortest path problem on an oriented graph, but requires the use of the vector of costs w in the input space.