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Support Vector Regression for the simultaneous learning of a multivariate function and its derivatives ☆

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Abstract

In this paper, the problem of simultaneously approximating a function and its derivatives is formulated within the Support Vector Machine (SVM) framework. First, the problem is solved for a one-dimensional input space by using the ε-insensitive loss function and introducing additional constraints in the approximation of the derivative. Then, we extend the method to multi-dimensional input spaces by a multidimensional regression algorithm. In both cases, to optimize the regression estimation problem, we have derived an iterative re-weighted least squares (IRWLS) procedure that works fast for moderate-size problems. The

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proposed method shows that using the information about derivatives significantly improves the reconstruction of the function.

Keywords: SVM; IRWLS

1. Introduction

Regression approximation of a given data set is a very common problem in a number of applications. In some of these applications, like economy, device modeling, telemetry, etc., it is necessary to fit not only the underlying characteristic function but also its derivatives, which are often available. The problem of learning a function and its derivatives has been addressed, for instance, in the neural networks literature, to analyze the capability of several kinds of networks [2,3], or in some applications [6,7]. Some other methods have been employed to simultaneously approximate a set of samples of a function and its derivative: splines, or filter bank-based methods are some examples (see [4] and references therein).

On the other hand, Support Vector Machines (SVMs) are state-of-the-art tools for linear and nonlinear input–output knowledge discovery [13,15]. The SVMs, given a labeled data set $(\mathbf{x}_i, y_i)$, where $\mathbf{x}_i \in \mathbb{R}^d$ for $i = 1, \ldots, N$, and a function $\boldsymbol{\phi}(\cdot)$ that nonlinearly transforms the input vector $\mathbf{x}_i$ to a higher-dimensional space, solve either classification ($y_i \in \{\pm 1\}$) or regression ($y_i \in \mathbb{R}$) problems.

In this paper, we will deal with the regression approximation problem and we will extend the SVM framework when prior knowledge regarding the derivatives of the functional relationship between $\mathbf{x}$ and y is known.

First, we will solve the issue in a one-dimensional problem ($d = 1$) by using the ε-insensitive loss function and introducing a linear constraint for the derivatives. Then, we will extend the method to multidimensional input spaces. In both cases, the corresponding method will lead to a solution similar to the SVM in which we have support vectors related to the function value and support vectors related to the derivatives values. Together, both kinds of support vectors form the complete SVM expansion for regression approximation with information about the derivatives of the function. The solution to the proposed algorithms is obtained using an iterative re-weighted least squares (IRWLS) procedure, which has been successfully applied to the regular SVM for classification [12] and for regression [11]. This algorithm has been recently proven to converge to the SVM solution [9].

2. Proposed one-dimensional SVM-based approach

The one-dimensional problem can be stated as follows: to find the functional relation between x and y giving a labeled data set, (x_i, y_i, y_i'), where $y_i \in \mathbb{R}$ and $y_i' \in \mathbb{R}$ is the derivative of the function to be approximated at x_i. The proposed method is an