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Recent Advances in Nonlinear Optimization and Equilibrium Problems: a Tribute to Marco D'Apuzzo

edited by Valentina De Simone, Daniela di Serafino, and Gerardo Toraldo

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A Convergent Hybrid Decomposition Algorithm Model Using Second Order Information for SVM Training: 49M27, 90C30.

Preface

This volume of *quaderni di matematica* is devoted to the memory of Marco D'Apuzzo, who died suddenly at the age of 46 in June of 2009.

Marco studied Mathematics at the University of Naples Federico II, where he also received his PhD in Applied Mathematics and Computer Science. His early scientific work dealt mainly with numerical linear algebra and parallel computing, during his years at the Department of Mathematics and its Applications at the University of Naples Federico II.

In 1999 he moved to the Department of Mathematics of the Second University of Naples, first as assistant professor and then as associate professor of numerical analysis, where he found his professional fulfilment. His research turned toward the numerical optimization field, in which Marco brought his passion and care for the computational aspects of numerical analysis, that were a constant throughout his scientific activity. With his colleagues at the Second University of Naples, who shared with him a well-established expertise in numerical linear algebra and numerical software design, he focused on the effective use of numerical linear algebra in the nonlinear optimization field. This activity was motivated by the simple observation that the effectiveness of any code for large-scale optimization depends heavily on the availability of effective linear algebra algorithms and software, since the overall computational effort is dominated by the solution of linear systems or the updating of matrix information. More specifically, Marco was interested in the linear algebra problems arising in interior point methods, and most of his late work was devoted to this topic. One of his last papers, entitled "On mutual impact of numerical linear algebra and large-scale optimization with focus on interior point methods", co-authored by Valentina De Simone and Daniela di Serafino, was posthumously awarded as COAP 2010 Best Paper (Computational Optimization and Applications, vol. 45, pp. 283-310).

His research was carried out within several national projects, with significant roles of responsibility, in which he was appreciated for his scientific and human qualities by his colleagues from all over the country, who demonstrate their respect and fondness for him with their commitment to this editorial project.

Marco also gave great service to his department, serving on various committees and especially as Math Course Coordinator, showing great kindness, enthusiasm and generosity toward students and colleagues, as well as ability to mediate among different positions.

In conclusion, during his too-short life, Marco proved to be not only a creative and productive scholar and teacher, but also a great person, for his cheerfulness, friendliness and generosity, and this book wants to be an homage from his friends in the Italian optimization community.

This volume includes thirteen invited papers from recognized experts in nonlinear optimization and equilibrium problems, covering a broad range of topics, from computational issues to more theoretical subjects, whose common denominator is the high quality of the contributions as well as the final goal of designing effective algorithms. In this sense, the spirit of this volume perfectly agrees with Marco's belief that the role of applied mathematics is to build effective tools able to provide solutions to problems in a wide range of applications.

The editors are indebted to the authors of the papers in this volume, who took much time from their busy schedules to put together a set of outstanding contributions. A special thanks goes to the eminent referees who gave a remarkable support in the review process, which was thorough and demanding, leading this editorial project to success.

We really miss the friend, the colleague, and the man.

Valentina De Simone, Daniela di Serafino, Gerardo Toraldo

Two-sphere Separation Procedures via Non-smooth Optimization

Annabella Astorino, Immanuel M. Bomze, Maria Paula Brito, and Manlio Gaudioso

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2. The two-sphere separation model (5).
3. Kernel transformation (9).
4. Conclusions (13).

1. Introduction and notation

Pattern analysis plays a central role in many modern artificial intelligence and computer science problems. The task is to detect regularities that characterize the data coming from a particular source, and the final objective is to design a system capable to make predictions about new data coming from the same source. Pattern analysis may lead to state a number of different problems such as classification, regression, cluster analysis, feature extraction, etc..

In particular the objective of pattern classification is to find a rule based on external observations to assign an object to exactly one among several classes. Many algorithms have been indeed devised for automatically classify several samples on the basis of their patterns. We mention here the pioneering contributions by Rosen [17], Mangasarian [15] and Bennett and Mangasarian [6].

The kernel method approach, leading to the introduction of the Support Vector Machine (SVM) [23, 18, 8], has been considered a real breakthrough in this area. The basic ideas of SVMs for classification problems are to map the data into a higher dimensional space (the feature space) and to separate the transformed sets by means of a hyperplane. Such a transformation finally provides a general nonlinear separation surface in the original input space (see [23, 18, 8] for an extensive treatment of the subject, and [10, 16] for effective variants). It is possible, however, to look for nonlinear separation surfaces directly in the input space, this is the case of the polyhedral separation [3] and of the ellipsoidal separation [4], or even in the feature space, as in the case of the spherical separation [5]. See [13, 14] for the numerical treatment of some semi-definite programming problems arising in set separation by means of a convex quadratic surface.

In this paper we are interested in the construction of spherical classifiers, where the objective is to partition either the input or the feature space into two different regions by using two spheres and to assign objects to their corresponding classes. We cite here Cooper's paper [7], where the design of spherical classifiers is strongly motivated for wide classes of data distributions.

Starting from the support vector data description (SVDD) method [20, 21] and building on the spherical separation with fixed center approach introduced in [5], we propose a new classification method based on the construction of two separation balls centered at appropriate points of the convex hulls of the classes we want to discriminate. By defining a suitable classification error function, we come out with a convex nonsmooth optimization problem, which can be solved by specialized methods such as bundle ones [11]. As in [5], the proposed approach can be used in connection with kernel transformations of the type adopted in the SVM approach.

The use of a couple of spheres appears advisable whenever the two classes should be treated in a similar way. This symmetry cannot be represented in the single-sphere classification approach. Moreover outliers detection seems more immediate in the two-spheres approach.

We observe that nonsmooth optimization theory plays a central role in the development of our supervised data classification algorithm. In fact, nonsmooth optimization has been successfully employed in several recent approaches to supervised and semi-supervised machine learning problems (see [2, 1]).

The paper is organized as follows. In section 1 we present first the two-sphere basic approach and then we introduce two variants. In the first one we move to the objective function one of the constraints of the basic model. In the second one we introduce a technique to deal with possible outliers. In section 2 we describe the possibility of applying our approach in connection with kernel transformation. Some conclusions are drawn in section 3.

In the sequel, we adopt the following notation: $\mathbb{R}^n_+$ is the positive orthant of n-dimensional Euclidean space $\mathbb{R}^n$. Given a finite index set I, we denote by $\Delta^I = \left\{\mathbf{x} \in \mathbb{R}^I_+ : \sum_{i \in I} x_i = 1\right\}$ the standard simplex. With $^\top$ denoting transposition, we denote by $\|\mathbf{x}\| = \sqrt{\mathbf{x}^\top \mathbf{x}}$ the usual Euclidean norm. The ball of radius r centered in $\overline{\mathbf{x}}$ is $B_r(\overline{\mathbf{x}}) = \left\{\mathbf{x} \in \mathbb{R}^d : \|\mathbf{x} - \overline{\mathbf{x}}\| \leq r\right\}$. For any $a \in \mathbb{R}$, the nonnegative scalar a_+ will indicate $\max\{0, a\}$.