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MISCLASSIFICATION MINIMIZATION

by

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# Misclassification Minimization

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## Abstract

The problem of minimizing the number of misclassified points by a plane, attempting to separate two point sets with intersecting convex hulls in  $n$ -dimensional real space, is formulated as a linear program with equilibrium constraints (LPEC). This general LPEC can be converted to an exact penalty problem with a quadratic objective and linear constraints. A Frank-Wolfe-type algorithm is proposed for the penalty problem that terminates at a stationary point or a global solution. Novel aspects of the approach include: (i) A linear complementarity formulation of the step function that "counts" misclassifications, (ii) Exact penalty formulation without boundedness, nondegeneracy or constraint qualification assumptions, (iii) An exact solution extraction from the sequence of minimizers of the penalty function for a finite value of the penalty parameter for the general LPEC and an explicitly exact solution for the LPEC with uncoupled constraints, and (iv) A parametric quadratic programming formulation of the LPEC associated with the misclassification minimization problem.

## 1 Introduction

We consider the fundamental problem of machine learning of discriminating between the elements of two point sets  $A$  and  $B$  in the  $n$ -dimensional real space  $R^n$ . These sets are represented by the  $m \times n$  and  $k \times n$  matrices  $A$  and  $B$  respectively. When the convex hulls of  $A$  and  $B$  are disjoint, a single linear program [14, 4] or the classical iterative perceptron algorithm [20, 9] will obtain a separating plane in a finite number of steps. In the general and usual case of intersecting convex hulls, the perceptron algorithm merely obtains a bounded sequence of iterates [7]. However, the linear programming formulation [4] obtains an approximate separating plane that minimizes some norm of the distances of misclassified points to the approximate separating plane. Although this approach has been quite successful in important real world applications [18, 21] and in the training of neural networks [3], the approximate separating plane does not minimize the number of misclassified points, as do some machine learning approaches [19]. In neural networks [12], misclassification minimization is achieved by using the sigmoid error function  $\frac{1}{1 + e^{-\alpha x}}$ , with a positive  $\alpha$ , to approximate a step function. Hence, minimization of the sum of distances of misclassified points by a linear program is merely a surrogate for misclassification minimization. In the present work, we propose a precise mathematical programming formulation of the nonconvex problem of minimizing the number of misclassified points. This is done in Section 2 where we first propose a simple linear complementarity formulation of the step function (Lemma 2.1) and then use this result to formulate the misclassification minimization as a linear program with an equilibrium (linear complementarity) constraint (Proposition 2.2). This LPEC is an important special case

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of mathematical programs with equilibrium constraints (MPEC) [11, 1] studied comprehensively recently in [13]. Section 3 deals with methods for solving a general LPEC. We convert our LPEC to an exact penalty problem and show (Theorem 3.2) that for a finite value of the penalty parameter an exact solution of the LPEC is contained in a minimizer of the penalty problem. Corollary 3.3 shows how to extract an exact solution from two minimizers of the penalty function. In Algorithm 3.4 we show how to solve the bilinear program, that constitutes the penalty problem, by a Frank-Wolfe type algorithm and establish its convergence in Theorem 3.5. In Section 4 we specialize to an LPEC with uncoupled equilibrium constraints (LPUEC) (33) which covers the misclassification minimization problem (12). Theorem 4.1 gives an explicitly exact penalty solution of this problem without any boundedness assumption that was required for the less general Stackelberg problem [2]. We propose Algorithm 4.2 as a finite stepless partial Frank-Wolfe algorithm for solving this problem. Its finite termination to an exact solution or a stationary point is established in Theorem 4.3. This algorithm is proposed for the solution of the parametric quadratic programming reformulation (41) of the misclassification minimization problem (12). This quadratic reformulation is proposed in order to overcome the stationarity of the penalty function for (12) at certain feasible points. Section 5 of the paper concludes with some brief remarks.

A word about our notation now. For a vector  $x$  in the  $n$ -dimensional real space  $R^n$ ,  $x_+$  will denote the vector in  $R^n$  with components  $(x_+)_i := \max\{x_i, 0\}$ ,  $i = 1, \dots, n$ . Similarly  $x_*$  will denote the vector in  $R^n$  with components  $(x_*)_i := (x_i)_*$ ,  $i = 1, \dots, n$ , where  $(\cdot)_*$  is the step function defined in (4) below. The notation  $A \in R^{m \times n}$  will signify a real  $m \times n$  matrix. For such a matrix,  $A^T$  will denote the transpose while  $A_i$  will denote row  $i$ . For two vectors  $x$  and  $y$  in  $R^n$ ,  $xy$  will denote the scalar product, while  $x \perp y$  will denote  $xy = 0$ . A vector of ones in a real space of arbitrary dimension will be denoted by  $e$ . The notation  $\arg \min_{x \in S} f(x)$  will denote the set of minimizers of  $f(x)$  on the set  $S$ , while the notation  $\arg \text{vertex partial} \min_{x \in S} f(x)$  will denote the set of vertices of  $S$  that approximately minimize  $f$  on  $S$ , and in particular any vertex of  $S$  may be taken to be in this set. The empty set, as well as an empty vector will be denoted by  $\emptyset$ .

## 2 Misclassification Minimization as a Linear Program with Equilibrium Constraint (LPEC)

When the point sets  $\mathcal{A}$  and  $\mathcal{B}$ , represented by the  $m \times n$  and  $k \times n$  matrices  $A$  and  $B$  respectively have disjoint convex hulls, they can be strictly separated [14] by a plane

$$wx = \gamma \quad (1)$$

in  $R^n$  where  $w$  is some weight vector constituting the normal to the separating plane and  $\gamma$  locates the plane relative to the origin. The plane (1) separates the sets  $\mathcal{A}$  and  $\mathcal{B}$  by the strict inequalities

$$Aw > e\gamma, \quad e\gamma > Bw \quad (2)$$

where  $e$  is a vector of ones of appropriate dimension. The system (2), upon normalization, is equivalent to

$$Aw - e\gamma - e \geq 0, \quad -Bw + e\gamma - e \geq 0 \quad (3)$$

Inequalities (3) state that the points  $A_i$ ,  $i = 1, \dots, m$ , lie in the open halfspace  $\{x | xw > \gamma\}$  in  $R^n$ , while the points  $B_i$ ,  $i = 1, \dots, k$ , lie on the open halfspace  $\{x | xw < \gamma\}$  in  $R^n$ . If we define the step function  $(\cdot)_* : R \rightarrow R$  as

$$(\xi)_* = \begin{cases} 1 & \text{if } \xi > 0 \\ 0 & \text{if } \xi \leq 0, \end{cases} \quad (4)$$

then the system (3) is equivalent to

$$e(-Aw + e\gamma + e)_* + e(Bw - e\gamma + e)_* = 0 \quad (5)$$

In fact, the left-hand side of (5) **counts** the number of misclassified points. For the linearly separable case of nonintersecting convex hulls, no points are misclassified, and hence the equality in (5) is obtained. In the more general case where the sets of  $\mathcal{A}$  and  $\mathcal{B}$  have intersecting convex hulls, and thus are linearly inseparable, equation (5) can be replaced by the minimization problem

$$\min_{w, \gamma} e(-Aw + e\gamma + e)_* + e(Bw - e\gamma + e)_* \quad (6)$$

This problem has a zero minimum if and only if the plane  $xw = \gamma$  strictly separates the sets  $\mathcal{A}$  and  $\mathcal{B}$ . Otherwise this plane minimizes the number of misclassified points, that is it minimizes

$$c(w, \gamma) := \text{cardinality} \left\{ (i, j) \left| \begin{array}{l} A_i w - \gamma - 1 < 0, -B_j w + \gamma - 1 < 0 \\ 1 \leq i \leq m, 1 \leq j \leq k \end{array} \right. \right\} \quad (7)$$

We immediately note that (6) is always solvable since there exists only a finite number of twofold partitions of  $\mathcal{A} \cup \mathcal{B}$  that are linearly separable. Any such partition that minimizes the number of misclassified points solves (6). Our objective is to reduce (6) to a mathematical programming problem. To do that we begin by a representation of the step function (4) as a complementarity condition via the plus function  $()_+$  as follows.

**Lemma 2.1** *Characterization of the step function  $()_*$*  For  $r \in R^m$ ,  $u \in R^m$ ,  $a \in R^m$  and  $e$ , a vector of ones in  $R^m$  :

$$r = (a)_*, u = a_+ \iff \begin{pmatrix} r \\ u \end{pmatrix} = \begin{pmatrix} r - u + a \\ r + u - e \end{pmatrix}_+ \quad (8)$$

**Proof** The points  $(a)_*$  and  $(a)_+$  solve respectively the dual linear programs

$$\max_r \{ar \mid 0 \leq r \leq e\} \text{ and } \min_u \{eu \mid u \geq a, u \geq 0\} \quad (9)$$

The right hand side of the equivalence (8) is merely the Karush-Kuhn-Tucker necessary and sufficient optimality conditions for  $r$  and  $u$  to solve (9), where use has been made of the elementary equivalence

$$c = d_+ \iff c - d \geq 0, c \geq 0, c(c - d) = 0 \quad (10)$$

for  $c \in R^m$  and  $d \in R^m$ . □

We now combine Lemma 2.1 and the minimization problem (6) and make use of (10), to obtain the following misclassification minimization characterization.

**Proposition 2.2** *Misclassification Minimization as a Linear Program with Equilibrium Constraints (LPEC)* A plane  $xw = \gamma$  minimizes the number of misclassifications  $c(w, \gamma)$  as defined by (7) if and only if  $(w, \gamma, r, u, s, v)$  solves the following linear program with equilibrium constraints:

$$\begin{array}{l} \underset{w, \gamma, r, u, s, v}{\text{minimize}} \quad er + es \\ \text{subject to} \quad \begin{pmatrix} r \\ u \end{pmatrix} = \begin{pmatrix} r - u - Aw + e\gamma + e \\ r + u - e \end{pmatrix}_+, \begin{pmatrix} s \\ v \end{pmatrix} = \begin{pmatrix} s - v + Bw - e\gamma + e \\ s + v - e \end{pmatrix}_+ \end{array} \quad (11)$$

or equivalently

$$\begin{aligned}
& \underset{w, \gamma, r, u, s, v}{\text{minimize}} && er + es \\
& && u + Aw - e\gamma - e \geq 0 && v - Bw + e\gamma - e \geq 0 \\
& && r \geq 0 && s \geq 0 \\
\text{subject to} &&& r(u + Aw - e\gamma - e) = 0 && s(v - Bw + e\gamma - e) = 0 \\
& && -r + e \geq 0 && -s + e \geq 0 \\
& && u \geq 0 && v \geq 0 \\
& && u(-r + e) = 0 && v(-s + e) = 0
\end{aligned} \tag{12}$$

We note that problem (12) is a linear program with equilibrium (linear complementarity) constraints (LPEC) and is a special case of the more general mathematical program with equilibrium constraints (MPEC) studied in detail by Luo, Pang, Ralph and Wu [13]. Being linear, our problem is endowed with some features not possessed by the more general MPECs, principally exactness of a penalty formulation without boundedness of the feasible region and without assuming nondegeneracy. We discuss these properties and an algorithm for solving (12) in the next section.

### 3 Linear Programs with Equilibrium Constraints (LPEC)

We consider the general LPEC

$$\begin{aligned}
& \underset{x, y}{\text{minimize}} && cx + dy \\
& && Mx + Ny + q \geq 0 \\
\text{subject to} &&& x(Mx + Ny + q) = 0 \\
& && x, y \geq 0
\end{aligned} \tag{13}$$

where  $M \in R^{\ell_1 \times \ell_1}$  and  $N \in R^{\ell_1 \times \ell_2}$ . Our misclassification minimization problem (12) is exactly of this type if we make the identification

$$x = \begin{pmatrix} r \\ u \\ s \\ v \end{pmatrix}, \quad y = \begin{pmatrix} t \\ \delta \\ \xi \end{pmatrix}, \quad \begin{pmatrix} w \\ \gamma \end{pmatrix} = \begin{pmatrix} t - e\xi \\ \delta - \xi \end{pmatrix}, \quad M = \begin{pmatrix} 0 & I & 0 & 0 \\ -I & 0 & 0 & 0 \\ 0 & 0 & 0 & I \\ 0 & 0 & -I & 0 \end{pmatrix}, \tag{14}$$

$$N = \begin{pmatrix} A & -e & -Ae + e \\ 0 & 0 & 0 \\ -B & e & Be - e \\ 0 & 0 & 0 \end{pmatrix}, \quad c = \begin{pmatrix} e \\ 0 \\ e \\ 0 \end{pmatrix}, \quad d = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad q = \begin{pmatrix} -e \\ e \\ -e \\ e \end{pmatrix}$$

We note that in (14),  $M + M^T = 0$ . Hence  $M$  is a skew symmetric positive semidefinite matrix, reflecting its linear programming origin (9). We also note that the linear objective function of (13) is bounded below by zero on the nonempty feasible region when the identifications (14) are made. This motivates the following simple existence results for (13).

**Theorem 3.1** *Existence of Solution for LPEC* A solution to (13) exists if it is feasible and its objective function is bounded below on its nonempty feasible region.

**Proof** The nonempty feasible region of (13) consists of the union of a finite number of polyhedral sets in  $R^{\ell_1 + \ell_2}$ . Since  $cx + dy$  is bounded below on each of these polyhedral sets it attains its minimum on each of them and its global minimum on their union.  $\square$

We now convert the LPEC (13) into a penalty problem of minimizing a quadratic function on a polyhedral set and show that for sufficiently large but finite value of the penalty parameter an exact solution can be identified. For that purpose it is convenient to define the following constraint sets:

$$\begin{aligned} S &:= \{(x, y) | Mx + Ny + q \geq 0, (x, y) \geq 0, x(Mx + Ny + q) = 0\} \\ S_0 &:= \{(x, y) | Mx + Ny + q \geq 0, (x, y) \geq 0\} \end{aligned} \quad (15)$$

We also define the following penalty function

$$P((x, y), \alpha) := cx + dy + \alpha x(Mx + Ny + q), \alpha \geq 0 \quad (16)$$

We will now show that for  $\alpha \geq \bar{\alpha}$ , for some  $\bar{\alpha} > 0$ , minimizing  $P((x, y), \alpha)$  over  $S_0$  will identify an exact solution of the LPEC (13). We state this result as follows.

**Theorem 3.2 *Exactness of LPEC Penalization*** *Let the feasible region  $S$  be nonempty and let  $cx + dy$  be bounded below on  $S_0$  of (15). There exists  $\bar{\alpha} > 0$  such that for any fixed  $\alpha \geq \bar{\alpha}$*

$$\begin{bmatrix} x(\alpha) \\ y(\alpha) \end{bmatrix} = \begin{bmatrix} \frac{a^i}{\alpha} + x_0^i \\ \frac{b^i}{\alpha} + y_0^i \end{bmatrix}, \text{ for some } i \in \{1, \dots, \ell\}, \quad (17)$$

where

$$(x(\alpha), y(\alpha)) \in \arg \min_{(x, y) \in S_0} P((x, y), \alpha) \quad (18)$$

Here  $\ell$  and the vectors  $a^i, b^i, x_0^i, y_0^i, i = 1, \dots, \ell$ , depend on the LPEC problem data only:  $M, N, C, d$  and  $q$ . Furthermore  $(x_0^i, y_0^i), i = 1, 2, \dots, \ell$ , solve the LPEC (13) and such that for any fixed  $\alpha \geq \bar{\alpha}$

$$x(\alpha)(Mx(\alpha) + Ny(\alpha) + q) = \frac{a^i(Ma^i + Nb^i)}{\alpha^2}, \text{ for some } i \in \{1, \dots, \ell\} \quad (19)$$

**Proof** First note that  $cx + dy$  is bounded below on  $S_0$  and  $x(Mx + Ny + q) \geq 0$  on  $S_0$ . It follows that the penalty problem of (18) is solvable by some  $(x(\alpha), y(\alpha))$  for each  $\alpha \geq 0$ . Hence for  $\alpha > 0$ ,  $x(\alpha), y(\alpha)$  and some  $u(\alpha) \in R^{\ell_1}$  satisfy the following Karush-Kuhn-Tucker conditions for (18)

$$0 \leq \begin{pmatrix} x \\ y \\ u \end{pmatrix} \perp \begin{pmatrix} (M + M^T) & N & -M^T \\ N^T & 0 & -N^T \\ M & N & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ u \end{pmatrix} + \begin{pmatrix} \frac{c}{\alpha} + q \\ \frac{d}{\alpha} \\ q \end{pmatrix} \geq 0 \quad (20)$$

The linear complementarity problem (20) has a vertex solution [16, Lemma 2], and hence a basic solution, for each  $\alpha > 0$ . Since (20) has a finite number of bases, it follows that on the set  $\{\alpha | \alpha \geq \bar{\alpha}\}$ , for some  $\bar{\alpha} > 0$ , only a finite number of basic solutions of (20) appear infinitely often, and no other basic solution appears a finite number of times. Denote the inverses of these  $(2\ell_1 + \ell_2) \times (2\ell_1 + \ell_2)$  matrices by

$$B^1, B^2, \dots, B^\ell \quad (21)$$

Then

$$\begin{bmatrix} x(\alpha) \\ y(\alpha) \\ u(\alpha) \end{bmatrix} = B^i \begin{bmatrix} \frac{c}{\alpha} + q \\ \frac{d}{\alpha} \\ q \end{bmatrix}, \quad i \in \{1, \dots, \ell\}, \quad \alpha \geq \bar{\alpha} \quad (22)$$

It follows from Theorem 2.8 of [17] by letting  $\alpha \rightarrow \infty$ , that

$$\begin{bmatrix} x_0^i \\ y_0^i \end{bmatrix} := \begin{bmatrix} x(\infty) \\ y(\infty) \end{bmatrix} := \begin{bmatrix} B_1^i \\ B_2^i \end{bmatrix} \begin{bmatrix} q \\ 0 \\ q \end{bmatrix}, \quad i \in \{1, \dots, \ell\}, \quad (23)$$

solve LPEC (13). This establishes (17) with  $\begin{bmatrix} a^i \\ b^i \end{bmatrix} = \begin{bmatrix} B_1^i \\ B_2^i \end{bmatrix} \begin{bmatrix} c \\ d \\ 0 \end{bmatrix}$  and  $\begin{bmatrix} x_0^i \\ y_0^i \end{bmatrix}$  as given by (23).

To establish (19) we employ Theorem 2.8 [17] again which states that

$$\lim_{\alpha \rightarrow \infty} \alpha x(\alpha)(Mx(\alpha) + Ny(\alpha) + q) = 0 \quad (24)$$

Since

$$x(\alpha)(Mx(\alpha) + Ny(\alpha) + q) = \frac{a^i g^i}{\alpha^2} + \frac{a^i h^i + x_0^i g^i}{\alpha} + x_0^i h^i, \quad i \in \{1, \dots, \ell\} \quad (25)$$

where

$$g^i := Ma^i + Nb^i, \quad h^i := Mx_0^i + Ny_0^i + q, \quad i \in \{1, \dots, \ell\} \quad (26)$$

It follows from (24) and (25) that

$$x_0^i h^i = 0 \quad \text{and} \quad a^i h^i + x_0^i g^i = 0, \quad i \in \{1, \dots, \ell\} \quad (27)$$

Combining (25) and (27) gives (19).  $\square$

With the help of Theorem 3.2, an exact solution of LPEC (13) can be recovered from (23) as follows.

**Corollary 3.3** *Let  $\alpha_2 > \alpha_1 \geq \bar{\alpha} > 0$  be such that the corresponding basic solutions  $(x(\alpha_2), y(\alpha_2), u(\alpha_2))$  and  $(x(\alpha_1), y(\alpha_1), u(\alpha_1))$  of (22) have the same basis  $B^i$ . Then  $(x_0^i, y_0^i)$  solves LPEC (13) where*

$$x_0^i = \frac{\alpha_2 x(\alpha_2) - \alpha_1 x(\alpha_1)}{\alpha_2 - \alpha_1} \quad (28)$$

$$y_0^i = \frac{\alpha_2 y(\alpha_2) - \alpha_1 y(\alpha_1)}{\alpha_2 - \alpha_1} \quad (29)$$

**Proof** From (17), since  $\alpha_2$  and  $\alpha_1$  generate solutions with the same basis it follows that

$$x(\alpha_1) = \frac{a^i}{\alpha_1} + x_0^i \quad (30)$$

$$x(\alpha_2) = \frac{a^i}{\alpha_2} + x_0^i \quad (31)$$

Subtracting (30) from (31) and solving  $a^i$  we get

$$a^i = \alpha_1 \alpha_2 \frac{x(\alpha_1) - x(\alpha_2)}{\alpha_2 - \alpha_1}$$

Substituting for  $\alpha^i$  in (30) gives (28). The expression (29) for  $y_0$  is similarly obtained.  $\square$

Corollary 3.3 is useful in obtaining an exact solution of LPEC (13) by monitoring repeated bases for  $\alpha \geq \bar{\alpha}$ , and using (28)-(29) to get the desired solution. Therefore, it remains to prescribe an algorithm for solving the penalty problem (18) for  $\alpha$  sufficiently large. We propose a Frank-Wolfe algorithm [10, 6] for solving (18) similar to that employed in [5]. This approach was quite successful in solving the nonconvex bilinear separability problem on many test cases [5]. For completeness we give the algorithm here. For convenience, however, we first define  $P(z, \alpha)$  as the penalty function of (16), that is

$$P(z, \alpha) := cx + dy + \alpha x(Mx + Ny + q), \quad z = \begin{pmatrix} x \\ y \end{pmatrix} \quad (32)$$

**Algorithm 3.4** *Frank-Wolfe Algorithm for Solving (18)* Fix  $\alpha > 0$ . Start with any  $z^0 \in S^0$ . Determine  $z^{j+1}$  from  $z^j$  as follows.

- $\bar{z}^j \in \arg \min_{z \in S^0} \nabla_z P(z^j, \alpha)z$
- Stop if  $\nabla_z P(z^j, \alpha)(\bar{z}^j - z^j) = 0$
- $z^{j+1} = (1 - \lambda^j)z^j + \lambda^j \bar{z}^j$ , where  $\lambda^j \in \arg \min_{0 \leq \lambda \leq 1} P(((1 - \lambda)z^j + \lambda \bar{z}^j), \alpha)$

Convergence of this algorithm is established in [5] without any convexity assumption on  $P(z, \alpha)$ . We state this convergence result without proof here.

**Theorem 3.5** *Convergence of Frank-Wolfe Algorithm* Algorithm 3.4 terminates at some  $z^j$  that satisfies the minimum principle necessary optimality condition:  $\nabla_z P(z^j, \alpha)(z - z^j) \geq 0$  for all  $z \in S^0$ , or each accumulation point  $\bar{z}$  of the sequence  $\{z^j\}$  satisfies the minimum principle.

## 4 Linear Programs with Uncoupled Equilibrium Constraints (LPUEC)

In this section we specialize the general LPEC (13) to the case of uncoupled equilibrium constraints, that is

$$\begin{aligned} & \underset{x, y}{\text{minimize}} && c_1 x_1 + c_2 x_2 + d_1 y_1 + d_2 y_2 \\ & && M_{12} x_2 + N_{11} y_1 + q_1 \geq 0 \\ & && M_{21} x_1 + N_{22} y_2 + q_2 \geq 0 \\ & \text{subject to} && x_1(M_{12} x_2 + N_{11} y_1 + q_1) = 0 \\ & && x_2(M_{21} x_1 + N_{22} y_2 + q_2) = 0 \\ & && x_1, x_2, y_1, y_2 \geq 0 \end{aligned} \quad (33)$$





where

$$x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, y = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}, c = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}, d = \begin{pmatrix} d_1 \\ d_2 \end{pmatrix}, q = \begin{pmatrix} q_1 \\ q_2 \end{pmatrix}, \quad (36)$$

$$M = \begin{pmatrix} 0 & M_{12} \\ M_{21} & 0 \end{pmatrix}, N = \begin{pmatrix} N_{11} & 0 \\ 0 & N_{22} \end{pmatrix}$$

$$P((x, y), \alpha) := cx + dy + \alpha x(Mx + Ny + q) \quad (37)$$

$$S := \{(x, y) | M\alpha + Ny + q \geq 0, (x, y) \geq 0, x(Mx + Ny + q) = 0\} \quad (38)$$

$$S_0 := S_{01} \times S_{02}$$

$$S_{01} := \{(x_2, y_1) | M_{12}x_2 + N_{11}y_1 + q_1 \geq 0, (x_2, y_1) \geq 0\} \quad (39)$$

$$S_{02} := \{(x_1, y_2) | M_{21}x_1 + N_{22}y_2 + q_2 \geq 0, (x_1, y_2) \geq 0\}$$

We show first that as a consequence of the fact that  $S_0 = S_{01} \times S_{02}$ , the penalty problem (35) always has a vertex solution and that for sufficiently large  $\alpha$ , an exact solution of LPUEC (33) is obtained.

**Theorem 4.1 *Explicit Exactness of LPUEC Penalization*** *Let LPUEC (33) have a nonempty feasible region  $S$ , and let its objective function be bounded below on  $S_0$ . Then*

(i) *LPUEC (33) has a solution which is a vertex of  $S_0$ .*

(ii) *For  $\alpha \geq \bar{\alpha}$  for some  $\bar{\alpha} > 0$ , the penalty function  $P((x, y), \alpha)$  attains a minimum on  $S_0$  at  $(\bar{x}, \bar{y})$  which is a vertex of  $S_0$  and a solution of LPUEC (33).*

**Proof** Note that (ii) implies (i) and hence we need only establish the latter.

We establish first that  $\min_{(x, y) \in S_0} P((x, y), \alpha)$  has a vertex solution for each  $\alpha \geq 0$ . Since  $cx + dy$  is bounded below on  $S_0$  by assumption, and  $x(Mx + Ny + q) \geq 0$  on  $S_0$ , it follows that the quadratic penalty function  $P((x, y), \alpha)$  has a minimum solution  $(\bar{x}(\alpha), \bar{y}(\alpha))$  in the polyhedral set  $S_0$  for  $\alpha \geq 0$  [10]. Hence the linear program

$$\min_{(x_2, y_1) \in S_{01}} P(((\bar{x}_1(\alpha), x_2), (y_1, \bar{y}_2(\alpha))), \alpha)$$

has a vertex  $(x_2(\alpha), y_1(\alpha))$  of  $S_{01}$  as solution and such that

$$P(((\bar{x}_1(\alpha), x_2(\alpha)), (y_1(\alpha), \bar{y}_2(\alpha))), \alpha) = P((\bar{x}(\alpha), \bar{y}(\alpha)), \alpha)$$

Similarly, the linear program

$$\min_{(x_1, y_2) \in S_{02}} P(((x_1, x_2(\alpha)), (y_1(\alpha), y_2)), \alpha)$$

has a vertex  $(x_1(\alpha), y_2(\alpha))$  of  $S_{02}$  as solution and such that

$$P((x(\alpha), y(\alpha)), \alpha) = P((\bar{x}_1(\alpha), x_2(\alpha), y_1(\alpha), \bar{y}_2(\alpha)), \alpha) = P((\bar{x}(\alpha), \bar{y}(\alpha)), \alpha)$$

Hence  $((x_2(\alpha), y_1(\alpha)), (x_1(\alpha), y_2(\alpha)))$  is a vertex of  $S_{01} \times S_{02}$  and consequently a vertex solution of  $\min_{(x,y) \in S_0} P((x, y), \alpha)$ .

We now establish exactness of the penalty problem  $\min_{(x,y) \in S_0} P((x, y), \alpha)$ . Let

$$(x(\alpha), y(\alpha)) \in \arg \text{vertex} \min_{(x,y) \in S_0} P((x, y), \alpha) \quad \text{for } \alpha \geq 0$$

Since  $S_0$  has a finite number of vertices, one vertex, say  $(\bar{x}, \bar{y})$  will satisfy

$$(\bar{x}, \bar{y}) \in \arg \text{vertex} \min_{(x,y) \in S_0} P((x, y), \alpha) \quad \alpha \geq \bar{\alpha} > 0$$

for some  $\bar{\alpha} > 0$ . By Theorem 2.5 [17] we have that

$$\bar{x}(M\bar{x} + N\bar{y} + q) = 0$$

Consequently, for all  $(x, y) \in S$  and  $\alpha \geq \bar{\alpha}$

$$c\bar{x} + d\bar{y} = P((\bar{x}, \bar{y}), \alpha) \leq P((x, y), \alpha) = cx + dy$$

Hence  $(\bar{x}, \bar{y})$  solves LPUEC (33). □

We now give a finite algorithm for solving LPUEC (33) that terminates either at a global solution or a point satisfying the minimum principle necessary optimality condition [15] for  $\min_{(x,y) \in S_0} P((x, y), \alpha)$ .

The algorithm consists of partially solving a succession of linear programs, and as such can be considered as a stepless Frank-Wolfe algorithm [10]. The ideas are similar to those of Algorithm 2.1 [5] for separable bilinear programs.

**Algorithm 4.2 Stepless Partial Frank-Wolfe for LPUEC (33)** For  $\alpha > 0$  start with  $(x^0, y^0) \in S$ . Determine  $(x^{i+1}, y^{i+1})$  from  $(x^i, y^i)$  as follows:

$$(x_2^{i+1}, y_1^{i+1}) \in \arg \text{vertex partial} \min_{(x_2, y_1) \in S_{01}} P(((x_1^i, x_2), (y_1, y_2^i)), \alpha)$$

$$(x_1^{i+1}, y_2^{i+1}) \in \arg \text{vertex partial} \min_{(x_1, y_2) \in S_{02}} P(((x_1, x_2^{i+1}), (y_1^{i+1}, y_2)), \alpha)$$

and such that  $P((x^{i+1}, y^{i+1}), \alpha) < P((x^i, y^i), \alpha)$ . Stop when impossible.

We establish now finite termination of Algorithm 4.2

**Theorem 4.3 Finite Termination of Algorithm 4.2** Let LPUEC (33) have a nonempty feasible region  $S$ , and let its objective function be bounded below on  $S_0$ . For  $\alpha \geq \bar{\alpha}$  for some  $\bar{\alpha} > 0$ , Algorithm 4.2 terminates in a finite number of steps at a solution of LPUEC (33) or at a point  $(x_1^i, x_2^{i+1}, y_1^{i+1}, y_2^i)$  that satisfies the minimum principle necessary optimality condition [15] for  $\min_{(x,y) \in S_0} P((x, y), \alpha)$ :

$$P(((x_1^i, x_2), (y_1, y_2^i)), \alpha) \geq P(((x_1^i, x_2^{i+1}), (y_1^{i+1}, y_2^i)), \alpha) \leq P(((x_1, x_2^{i+1}), (y_1^{i+1}, y_2, )), \alpha), \forall (x, y) \in S_0 \quad (40)$$

**Proof** If for some  $i$ ,  $P((x^{i+1}, y^{i+1}), \alpha) \not\leq P((x^i, y^i), \alpha)$ , then each of the two linear programs of Algorithm 4.2 must have been solved to optimality, and  $P(((x_1^i, x_2^i), (y_1^i, y_2^i)), \alpha) \geq P((x^i, y^i), \alpha) = P(((x_1^i, x_2^{i+1}), (y_1^{i+1}, y_2^i)), \alpha) = P((x^{i+1}, y^{i+1}), \alpha) \leq P(((x_1, x_2^{i+1}), (y_1^{i+1}, y_2)), \alpha), \forall (x, y) \in S_0$ . From this the minimum principle (40) follows. Since there are a finite number of vertices of  $S_0 = S_{01} \times S_{02}$ , and since for each vertex visited by Algorithm 4.2 the penalty function  $P((x, y), \alpha)$ , strictly decreases, no vertex of  $S_0$  is repeated. Thus, Algorithm 4.2 terminates at  $(x_1^i, x_2^{i+1}, y_1^{i+1}, y_2^i)$  which is either a global minimum of  $P((x, y), \alpha)$  on  $S_0$  or  $(x_1^i, x_2^{i+1}, y_1^{i+1}, y_2^i)$  satisfies the minimum principle (40). In the former case, it follows by Theorem 4.1 that  $(x_1^i, x_2^{i+1}, y_1^{i+1}, y_2^i)$  solves LPUEC (33).  $\square$

We return now to the misclassification minimization problem (12). Curiously, it turns out that the penalty function (37) for (12), has a stationary point on  $S_0$  for each arbitrary  $(w, \gamma)$  defining the plane (1) and appropriately chosen  $(r, u, s, v)$ . We skip the algebra that shows this, but give an intuitive justification of this curious fact. This may also explain why optimization algorithms, including the classical backpropagation algorithm of neural networks [12], may be slow when applied directly to the misclassification error function of (6) or the equivalent formulation (12), instead of the parametric quadratic minimization (41) proposed below. Suppose that the plane  $wx = \gamma$  does not pass through any of the points of either set  $\mathcal{A}$  or  $\mathcal{B}$ . A small perturbation in either  $w$  or  $\gamma$  or both will not change the number of misclassified points. Hence for such  $(w, \gamma)$  and its perturbation, the constraints of (12), which merely generate  $r$  and  $s$  that count misclassifications, remain satisfied by the perturbed  $(w, \gamma)$  and some corresponding  $(r, u, s, v)$ , but the objective function  $er + es$  remains constant. Thus  $(w, \gamma)$  is stationary. To avoid this difficulty we consider the following parametric reformulation of problem (12)

$$\begin{aligned}
& \underset{w, \gamma, r, u, s, v}{\text{minimize}} && \frac{1}{m}[r(Aw - e\gamma - e) + eu] + \frac{1}{k}[s(-Bw + e\gamma - e) + ev] \\
& && u + Aw - e\gamma - e \geq 0 && v - Bw + e\gamma - e \geq 0 \\
& && r \geq 0 && s \geq 0 \\
\text{subject to} &&& -r + e \geq 0 && -s + e \geq 0 \\
& && u \geq 0 && v \geq 0 \\
& && && er + es \leq \delta \\
& && && \delta \in [0, \infty)
\end{aligned} \tag{41}$$

Here the weights  $\frac{1}{m}$  and  $\frac{1}{k}$  are used to average the complementarity condition over the cardinalities  $m$  and  $k$  of the sets  $\mathcal{A}$  and  $\mathcal{B}$  respectively. This is motivated by the fact that when  $\delta = 0$ , problem (41) reduces precisely to problem (2.11) of [4] which is guaranteed to generate a non-null  $w$  that will minimize the average of the distances of misclassified points (assuming  $\|A_i\|_2 = 1$ ,  $\|B_j\|_2 = 1$ ,  $i = 1, \dots, m$ ,  $j = 1, \dots, k$ ). Note that problem (41) is solvable for each  $\delta \in [0, \infty)$ , because its quadratic objective is bounded below on its nonempty feasible region [10]. Furthermore  $f(\delta)$ , the nonnegative minimum value of (41), is a nonincreasing function of  $\delta$  that decreases to zero at  $\delta = \bar{\delta}$ , for some  $\bar{\delta} \geq 0$ , which is the global minimum of problem (12). This is so, because the objective function of (41), which consists of the complementarity constraints of (12), becomes zero first at some  $\bar{\delta}$ , the smallest value of  $\delta$ , for which the constraints of (12) are satisfied and  $er + es$  is minimized, thus giving the smallest number of misclassified points. Hence problem (12) is reduced to solving problem (41) for  $\delta = \bar{\delta}$ , the smallest nonnegative root of  $f(\delta) = 0$ , that is

$$\bar{\delta} = \min_{\delta \geq 0} \{\delta \mid f(\delta) = 0\} \tag{42}$$

Obviously if  $\bar{\delta} = 0$ , then the sets  $\mathcal{A}$  and  $\mathcal{B}$  are linearly separable and no points are misclassified. Our proposed procedure is to solve (41) by Algorithm 4.2 for increasing values of  $\delta$  until  $f(\delta) = 0$ .

A one dimensional secant method [8] for finding a nonnegative root of  $f(\delta) = 0$  may be helpful. We note that  $f(\delta) = 0$  for  $\delta \geq \bar{\delta}$ .

## 5 Conclusion

We have formulated the problem of minimizing the number of misclassified points by a plane attempting to separate two point sets in  $R^n$  as a problem of minimizing of a nonconvex quadratic function subject to linear inequalities. The quadratic program is either a penalty problem with a finite value of the penalty parameter obtained from a linear program with equilibrium constraints (LPEC), or a parametric nonconvex quadratic minimization problem with linear constraints. Our exact penalty formulation of the general LPEC, both with coupled and uncoupled constraints, require no assumptions on the problem other than feasibility and boundedness from below on the objective function. These assumptions are automatically satisfied by the LPEC associated with the misclassification minimization.

When the constraints of the LPEC are coupled, our exact penalty formulation (16) requires some calculation to obtain an exact solution to the original LPEC. However, when the constraints are uncoupled as in (33), which is the case for the misclassification minimization problem (12), our exact penalty (16) directly yields an explicit solution to the LPEC for a finite value of the penalty parameter. The method that we propose for solving the misclassification minimization problem is the linear-programming-based Algorithm 4.2, applied to the parametric quadratic program (41) as a bilinear program. We think that this effective approach for solving the misclassification minimization problem is worthy of further study and numerical testing.

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