Feature selection via Mixed Integer Linear Programming

Martine Labbé   Antonio M. Rodríguez-Chía

Dept. Computer Science. Université Libre de Bruxelles
Dept. Statistics and Operations Research. Universidad de Cádiz (Sabbatical in ULB)

Contents:

Contents:

- Introduction to classification problems:
  - Classification problems via Mixed Integer Linear Programming.
  - Support Vector Machine.
  - Feature selection.
- A classification model with feature selection.
- Analysis of the model.

Supervised classification problem (discriminant analysis)

Given:

- Ω: set of objects.
- $\mathcal{C}$: predefined set of classes.

The aim is to build a classification rule that predicts the class membership of an object, $u \in \Omega$ into one of the class of $\mathcal{C}$ by means of its predictor $x^u \in \mathbb{R}^n$.

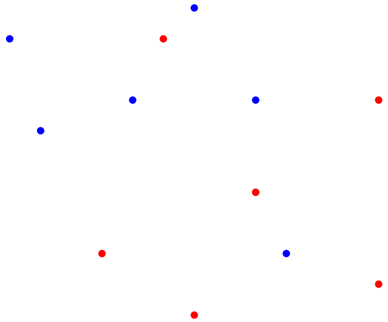
Applications:

- Biology and medicine: Classification of gene expression data, homology detection, cancer diagnosis.
- Agriculture.
- Business: credit scoring, fraud detection, bankrupty.

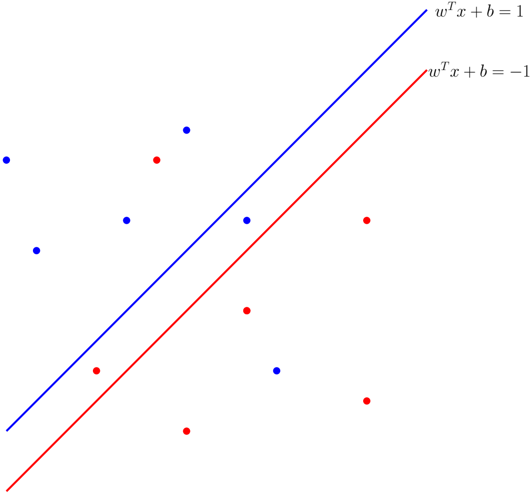
Support Vector Machine (Cortes and Vapnik (1995))

- $x_j \in \mathbb{R}^n$ training sample $j = 1, \ldots, m$.
- $y_j \in \{-1, +1\}$ their labels.
- $f(x) = w^T x + b$ a hyperplane to optimally separate the training sample.
- The SVM formulatation balances:
  - Structural risk or Margin: minimization of $\|w\|$.
  - Empirical risk or deviations: misclassification errors ξ.

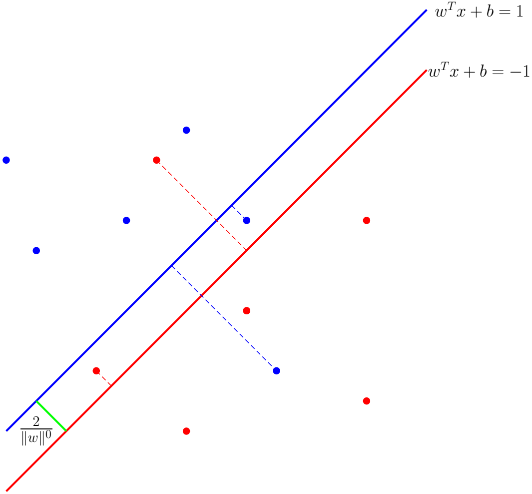
Support Vector Machine (Cortes and Vapnik (1995))



Support Vector Machine (Cortes and Vapnik (1995))



Support Vector Machine (Cortes and Vapnik (1995))



Support Vector Machine

$$\left.\begin{array}{ll} y_i = 1 & \Longrightarrow w^t x_i + b \geq 1 \\ y_i = -1 & \Longrightarrow w^t x_i + b \leq -1 \end{array}\right\} \Longrightarrow y_i(w^T x_i + b) \geq 1$$

ℓ_2 Support Vector Machine: Bradley and Mangasarian (1998)

$$\begin{array}{ll} \min_{w,b,\xi} & \|w\|_2 + C \sum_{i=1}^{m} \xi_i \\ s.t. & y_i(w^T x_i + b) \geq 1 - \xi_i, \quad \forall i = 1, \ldots, m, \\ & \xi_i \geq 0, \quad \forall i = 1, \ldots, m. \end{array}$$

Support Vector Machine

ℓ_1 Support Vector Machine (Bradley and Mangasarian (1998))

$$\begin{aligned} \min_{w,b,\xi} \quad & \|w\|_1 + C\sum_{i=1}^{m}\xi_i \\ s.t. \quad & y_i(w^T x_i + b) \geq 1 - \xi_i, \quad \forall i = 1, \ldots, m, \\ & \xi_i \geq 0, \quad \forall i = 1, \ldots, m. \end{aligned}$$

Or equivalently,

$$\begin{aligned} \min_{w,b,\xi} \quad & \sum_{j=1}^{n} z_j + C\sum_{i=1}^{m}\xi_i \\ s.t. \quad & y_i\Big(\sum_{j=1}^{m} w_j x_{ij} + b\Big) \geq 1 - \xi_i, \quad \forall i = 1, \ldots, m, \\ & -z_j \leq w_j \leq z_j, \quad \forall j = 1, \ldots, n, \\ & \xi_i \geq 0, \quad \forall i = 1, \ldots, m. \end{aligned}$$

Feature Selection

$$x = \begin{pmatrix} x_{11} & \dots & x_{1j} & \dots & x_{1n} \\ \vdots & \ddots & & & \vdots \\ x_{i1} & & x_{ij} & & x_{in} \\ \vdots & & & \ddots & \vdots \\ x_{m1} & \dots & x_{mj} & \dots & x_{mn} \end{pmatrix}$$

Usual case: $n >>> m$.

- Colorectal: 60×2000.
- Brain-Tumor1: 71×7131.
- Brain-Tumor2: 50×12627.
- Cancer I: 214×31099.
- Cancer II: 340×54675.

Support Vector Machine & Feature Selection

- Maldonado, Pérez, Labbé, Weber (2014)
- Feature selection via a budget constraint
- l_j/u_j correspond to a lower/upper bounds of the value of w_j, $\forall j$.

$$\begin{aligned}
\min_{w,b,\xi,v} \quad & \sum_{i=1}^{m} \xi_i \\
s.t. \quad & y_i\Big(\sum_{j=1}^{m} w_j x_{ij} + b\Big) \geq 1 - \xi_i, \quad \forall i = 1, \ldots, m, \\
& l_j v_j \leq w_j \leq u_j v_j, \quad \forall j = 1, \ldots, n, \\
& \sum_{j=1}^{m} v_j \leq B, \\
& v_j \in \{0,1\}, \quad \forall j = 1, \ldots, n, \\
& \xi_i \geq 0, \quad \forall i = 1, \ldots, m.
\end{aligned}$$

Support Vector Machine & Feature Selection

- Maldonado, Pérez, Labbé, Weber (2014)
- Feature selection via a budget constraint
- l_j/u_j correspond to a lower/upper bounds of the value of w_j, $\forall j$.

$$
\begin{aligned}
\min_{w,b,\xi,v} \quad & \sum_{i=1}^{m} \xi_i \\
s.t. \quad & y_i\Big(\sum_{j=1}^{m} w_j x_{ij} + b\Big) \geq 1 - \xi_i, \quad \forall i = 1, \ldots, m, \\
& l_j v_j \leq w_j \leq u_j v_j, \quad \forall j = 1, \ldots, n, \\
& \sum_{j=1}^{m} v_j \leq B, \\
& v_j \in \{0, 1\}, \quad \forall j = 1, \ldots, n, \\
& \xi_i \geq 0, \quad \forall i = 1, \ldots, m.
\end{aligned}
$$

An important issue is the appropriate choice of these bounds.

The model

$$
\begin{aligned}
\min_{w,b,\xi,v,z} \quad & \sum_{i=1}^{m} \xi_i + C \sum_{j=1}^{n} z_j \\
s.t. \quad & y_i \Big(\sum_{j=1}^{m} w_j x_{ij} + b \Big) \geq 1 - \xi_i, \quad \forall i = 1, \dots, m, \\
& l_j v_j \leq w_j \leq u_j v_j, \quad \forall j = 1, \dots, n, \\
& -z_j \leq w_j \leq z_j, \quad \forall j = 1, \dots, n, \\
& \sum_{j=1}^{m} v_j \leq B, \\
& v_j \in \{0, 1\},\ w_j \text{ unrestricted}, \quad \forall j = 1, \dots, n, \\
& \xi_i \geq 0, \quad \forall i = 1, \dots, m.
\end{aligned}
$$

The model

$$\min_{w,b,\xi,v,z} \quad \sum_{i=1}^{m} \xi_i + C \sum_{j=1}^{n} z_j$$

$$\begin{aligned}
s.t. \quad & y_i \Big(\sum_{j=1}^{m} w_j x_{ij} + b \Big) \geq 1 - \xi_i, \quad \forall i = 1, \ldots, m, \\
& l_j v_j \leq w_j \leq u_j v_j, \quad \forall j = 1, \ldots, n, \\
& -z_j \leq w_j \leq z_j, \quad \forall j = 1, \ldots, n, \\
& \sum_{j=1}^{m} v_j \leq B, \\
& v_j \in \{0, 1\}, \; w_j \text{ unrestricted}, \quad \forall j = 1, \ldots, n, \\
& \xi_i \geq 0, \quad \forall i = 1, \ldots, m.
\end{aligned}$$

For simplicity: $l_j = -u_j \; \forall j = 1, \ldots, n.$

Column Generation

$$\overbrace{y_i \sum_{j=1}^{m} x_{ij} w_j}^{A_1} + \overbrace{y_i b + \xi_i}^{A_2} \geq 1, \quad \forall i = 1, \ldots, m$$

$$\left.\begin{array}{ll} w_j \leq u_j v_j, & \forall j = 1, \ldots, n \\ -w_j \leq u_j v_j, & \forall j = 1, \ldots, n \\ w_j + z_j \geq 0, & \forall j = 1, \ldots, n \\ -w_j + z_j \geq 0, & \forall j = 1, \ldots, n \\ \sum_{j=1}^{n} v_j \leq B, & \\ v_j \in \{0, 1\}, & \end{array}\right\} X^1$$

$$\xi_i \geq 0, \forall i = 1, \ldots, m, \ b \text{ unrestricted} \quad \longrightarrow \quad X^0$$

Column Generation

$$\overbrace{y_i \sum_{j=1}^{m} x_{ij} w_j}^{A_1} + \overbrace{y_i b + \xi_i}^{A_2} \geq 1, \quad \forall i = 1, \ldots, m$$

$$\left.\begin{array}{ll} w_j \leq u_j v_j, & \forall j = 1, \ldots, n \\ -w_j \leq u_j v_j, & \forall j = 1, \ldots, n \\ w_j + z_j \geq 0, & \forall j = 1, \ldots, n \\ -w_j + z_j \geq 0, & \forall j = 1, \ldots, n \\ \sum_{j=1}^{n} v_j \leq B, & \\ v_j \in \{0, 1\}, & \end{array}\right\} X^1$$

$$\xi_i \geq 0, \forall i = 1, \ldots, m, \; b \text{ unrestricted} \quad \longrightarrow \quad X^0$$

Extreme points: $(v_j, w_j, z_j) = \{(0,0,0), (1, u_j, u_j), (1, -u_j, u_j)\}$

Column Generation

- $z_j = \sum_{t=1}^{T} \lambda^t z_j^t, \quad w_j = \sum_{t=1}^{T} \lambda^t w_j^t$

$$
\begin{aligned}
\min \quad & \sum_{i=1}^{m} \xi_i + C \sum_{t=1}^{T} \sum_{j=1}^{n} \lambda^t z_j^t \\
s.t. \quad & y_i \sum_{t=1}^{T} \sum_{j=1}^{n} x_{ij} w_j^t \lambda^t + y_i b + \xi_i \geq 1, \quad i = 1, \ldots, m \\
& \sum_{t=1}^{T} \lambda^t = 1, \\
& \lambda^t \geq 0, \quad t = 1, \ldots, T \\
& \xi_i \geq 0, \quad \forall i = 1, \ldots, m.
\end{aligned}
$$

Column Generation

Computation of the reduced cost:

$$\begin{aligned}
\min \quad & C\sum_{j=1}^{n} z_j - \sum_{i=1}^{m}\alpha_i y_i \sum_{j=1}^{n} w_j x_{ij} - \beta \\
s.t. \quad & w_j \geq -u_j v_j, \quad \forall j = 1, \ldots, n \\
& w_j \leq u_j v_j, \quad \forall j = 1, \ldots, n \\
& w_j + z_j \geq 0, \quad \forall j = 1, \ldots, n \\
& -w_j + z_j \geq 0, \quad \forall j = 1, \ldots, n \\
& \sum_{j=1}^{n} v_j \leq B, \\
& v_j \in \{0, 1\}, \quad \forall j = 1, \ldots, n.
\end{aligned}$$

Objective function:

$$\sum_{j=1}^{m} Cz_j - (\sum_{i=1}^{n}\alpha_i y_i x_{ij})w_j \sim \sum_{j=1}^{n} C|w_j| - (\sum_{i=1}^{n}\alpha_i y_i x_{ij})w_j.$$

Column Generation

Derivative of objective function with respect to w_j is:

$$\begin{array}{ll} C - \sum_{i=1}^n \alpha_i y_i x_{ij} & \text{if } w_j \geq 0 \\ -C - \sum_{i=1}^n \alpha_i y_i x_{ij} & \text{if } w_j \leq 0 \end{array}$$

- If $C > \sum_{i=1}^n \alpha_i y_i x_{ij}$ and $w_j \geq 0$ then $w_j^* = 0$.
- If $C < \sum_{i=1}^n \alpha_i y_i x_{ij}$ and $w_j \geq 0$ then $w_j^* = u_j$.
- If $C \leq -\sum_{i=1}^n \alpha_i y_i x_{ij}$ and $w_j \leq 0$ then $w_j^* = -u_j$.
- If $C \geq -\sum_{i=1}^n \alpha_i y_i x_{ij}$ and $w_j \leq 0$ then $w_j^* = 0$.

$\forall j = 1, \ldots, n$. Consider:

$$\left(\min \left\{ 0, C|u_j| - \sum_{i=1}^n \alpha_i y_i x_{ij} u_j, C|u_j| + \sum_{i=1}^n \alpha_i y_i x_{ij} u_j \right\} \right)_{j=1}^n =$$

$$\left(\min \left\{ 0, C - \sum_{i=1}^n \alpha_i y_i x_{ij}, C + \sum_{i=1}^n \alpha_i y_i x_{ij} \right\} \right)_{j=1}^n .$$

Choose the B smallest values.

The model

Reformulation: Formulation II.

Considering $w_j = w_j^a - w_j^b$, where $w_j^a, w_j^b \geq 0$, $\forall j = 1, \ldots, n$.

$$\begin{aligned}
\min_{w,b,\xi,v,z} \quad & \sum_{i=1}^{m} \xi_i + C \sum_{j=1}^{n} (w_j^a + w_j^b) \\
s.t. \quad & y_i \Big(\sum_{j=1}^{m} (w_j^a - w_j^b) x_{ij} + b \Big) \geq 1 - \xi_i, \quad \forall i = 1, \ldots, m, \\
& w_j^a + w_j^b \leq u_j v_j, \quad \forall j = 1, \ldots, n, \\
& \sum_{j=1}^{m} v_j \leq B, \\
& v_j \in \{0, 1\}, w_j^a, w_j^b \geq 0, \quad \forall j = 1, \ldots, n, \\
& \xi_i \geq 0, \quad \forall i = 1, \ldots, m.
\end{aligned}$$

Comparative:

	Form.-1	Col. Generat.	Form.-2
Leukemia1=72x5329	43.92	9.63	1.66
Brain-Tumor1=60x7131	65.69	2.61	1.97
DLBCL=77x7131	78.98	13.02	2.16
Carcinoma=36x7459	47.72	12.97	0.98
Brain-Tumor2=50x12627	233.49	13.09	2.30
Prostate-Tumor=102x12606	618.61	36.89	6.66

Strategy for obtaining tightened values of u_j

Strategy I:

Step 1: Solve the LP problem.

$$
\begin{aligned}
\min_{w,b,\xi,v,z} \quad & \sum_{i=1}^{m} \xi_i + C \sum_{j=1}^{n} (w_j^a + w_j^b) \\
s.t. \quad & y_i \Big(\sum_{j=1}^{m} (w_j^a - w_j^b) x_{ij} + b \Big) \geq 1 - \xi_i, \quad \forall i = 1, \ldots, m \\
& w_j^a + w_j^b \leq u_j v_j, \quad \forall j = 1, \ldots, n \\
& \sum_{j=1}^{m} v_j \leq B, \\
& 0 \leq v_j \leq 1, w_j^a, w_j^b \geq 0 \quad \forall j = 1, \ldots, n \\
& \xi_i \geq 0, \quad \forall i = 1, \ldots, m \\
& b \text{ unrestricted.}
\end{aligned}
$$

Strategy for obtaining tightened values of u_j

Strategy I:

Step 1: Solve the LP problem.

Step 2: Let $\overline{w}_j^a$ and $\overline{w}_j^b$ be the optimal solution and set $J_1 = \{j \,:\, \overline{w}_j^a + \overline{w}_j^b > 0\}$. Solve the following $MILP(J_1)$:

$$\begin{aligned}
\max_{w,b,\xi,v,z} \quad & \sum_{i=1}^{m} \xi_i + C \sum_{j \in J_1} (w_j^a + w_j^b) \\
s.t. \quad & y_i \Big(\sum_{j \in J_1} (w_j^a - w_j^b) x_{ij} + b \Big) \geq 1 - \xi_i, \quad \forall i = 1, \ldots, m \\
& w_j^a + w_j^b \leq u_j v_j, \quad \forall j \in J_1 \\
& \sum_{j \in J_1} v_j \leq B, \\
& v_j \in \{0,1\}, w_j^a, w_j^b \geq 0 \quad \forall j \in J_1, \\
& \xi_i \geq 0, \quad \forall i = 1, \ldots, m \\
& b \text{ unrestricted.}
\end{aligned}$$

Strategy for obtaining tightened values of u_j

Strategy I:

Step 1: Solve the LR problem.

Step 2: Let $J_1 = \{j \,:\, \overline{w}_j^a + \overline{w}_j^b > 0\}$. Solve t $MILP(J_1)$:

Step 3: Let UB be the optimal value of the above problem.

$$\begin{aligned}
\min_{w,b,\xi,v} \quad & w_j^a + w_j^b \\
s.t. \quad & y_i \Big(\sum_{j=1}^{m} (w_j^a - w_j^b) x_{ij} + b \Big) \geq 1 - \xi_i, \;\; \forall i = 1, \dots, m \\
& w_j^a + w_j^b \leq u_j v_j, \quad \forall j = 1, \dots, n \\
& \sum_{j=1}^{m} v_j \leq B, \\
& \sum_{i=1}^{m} \xi_i + C \sum_{j=1}^{n} (w_j^a + w_j^b) \leq UB, \\
& 0 \leq v_j \leq 1, w_j^a, w_j^b \geq 0 \,\forall j, \; \xi_i \geq 0, \; \forall i, \; b \text{ unrestricted.}
\end{aligned}$$

Strategy for obtaining tightened values of u_j

Strategy I:

Step 1: Solve the LR problem.

Step 2: Let $\overline{w}_j^a$ and $\overline{w}_j^b$ be the optimal solution and set $J_1 = \{j \, : \, \overline{w}_j^a + \overline{w}_j^b > 0\}$. Solve the following $MILP(J_1)$:

Step 3: Let *obval* be the optimal value of the above problem.

Output: Let $\overline{w}_j^a + \overline{w}_j^b$ be the optimal value of the above problem for $j = 1, \ldots, n$. Update the values of u_j as follows: If $\overline{w}_j^a + \overline{w}_j^b < u_j$ then $u_j := \overline{w}_j^a + \overline{w}_j^b$ for $j = 1, \ldots, n$.

Strategy for obtaining tightened values of u_j

Strategy II:

Step 1: Solve the LP problem.

$$\min_{w,b,\xi,v,z} \quad \sum_{i=1}^{m} \xi_i + C\sum_{j=1}^{n}(w_j^a + w_j^b)$$

$$s.t. \quad y_i\Big(\sum_{j=1}^{m}(w_j^a - w_j^b)x_{ij} + b\Big) \geq 1 - \xi_i, \quad \forall i = 1,\ldots,m$$

$$w_j^a + w_j^b \leq u_j v_j, \quad \forall j = 1,\ldots,n$$

$$\sum_{j=1}^{m} v_j \leq B,$$

$$0 \leq v_j \leq 1, w_j^a, w_j^b \geq 0 \quad \forall j = 1,\ldots,n$$

$$\xi_i \geq 0, \quad \forall i = 1,\ldots,m$$

b unrestricted.

Strategy for obtaining tightened values of u_j

Strategy II:

Step 1: Consider linear relaxation.

Step 2: LB:the optimal value of this problem

$w_j^{a^*}$, $w_j^{b^*}$: the optimal solutions.

If $w_{j_0}^{a^*} = 0$ and $w_{j_0}^{b^*} = 0$:

i) The optimum value of the problem with $w_{j_0}^a = \overline{w}_{j_0}^a$ is:

$$LB + \overline{w}_{j_0}^a \Big(C - \sum_{i=1}^{m} \alpha_i y_i x_{i j_0} \Big)$$

$$\text{whenever } \sum_{j=1}^{m} v_j^* + \frac{\overline{w}_{j_0}^a}{u_{j_0}} \leq B.$$

Step 3: Let UB be an upper bound of the objective function:

i) $LB + \overline{w}_{j_0}^a (C - \sum_{i=1}^{n} \alpha_i y_i x_{ij_0}) \leq UB$ then

$$\overline{w}_{j_0}^a \leq \frac{UB - LB}{C - \sum_{i=1}^{m} \alpha_i y_i x_{ij_0}}.$$

Strategy for obtaining tightened values of u_j

Strategy I: $\lvert w \rvert = w^a + w^b$	Strategy II: w^a, w^b
u(3)=0,537901	ua(3):=0,947904; ub(3):=0,280248
u(4)=0,455854	ua(4):=0,517722; ub(4):=0,371513
u(5)=0,556773	ua(5):=0,345003; ub(5):=0,579808
u(6)=0,441695	ua(6):=0,413056; ub(6):=0,45408
u(7)=0,436505	ua(7):=0,437826; ub(7):=0,427492
u(8)=0,456681	ua(8):=0,457311; ub(8):=0,410419
u(9)=0,43807	ua(9):=0,435321; ub(9):=0,429909
u(10)=0,470935	ua(10):=0,473788; ub(10):=0,397997
u(11)=0,45484	ua(11):=0,355108; ub(11):=0,553345
u(12)=0,436303	ua(12):=0,427289; ub(12):=0,43804
u(13)=0,462439	ua(13):=0,376622; ub(13):=0,508116
u(14)=0,610984	ua(14):=0,813715; ub(14):=0,294612
u(15)=0,587497	ua(15):=0,770599; ub(15):=0,300703
u(16)=0,628137	ua(16):=0,841183; ub(16):=0,291169

Flow cover inequalities

$$X = \{(x,y) \in \mathbb{R}^n_+ \times B^n \ : \ \sum_{j\in N_1} x_j - \sum_{j\in N_2} x_j \leq b, \ x_j \leq a_j y_j \text{ for } j \in N_1 \cup N_2\}.$$

Let $C = C_1 \cup C_2$ with $C_1 \subseteq N_1, \ C_2 \subseteq N_2$:

$$\sum_{j\in C_1} a_j - \sum_{j\in C_2} a_j = b + \lambda, \quad \lambda > 0.$$

$$\sum_{j\in C_1} x_j + \sum_{j\in C_1} (a_j - \lambda)^+ (1 - y_j) \leq b + \sum_{j\in C_2} a_j + \lambda \sum_{j\in L_2} y_j + \sum_{j\in N_2 \setminus (C_2 \cup L_2)} x_j.$$

A separation heuristic for the FCI by solving the following knapsack pb:

$$\begin{aligned} \min \quad & \sum_{j\in N_1} (1 - y_j^*) z_j - \sum_{j\in N_2} y_j^* z_j \\ s.t. \quad & \sum_{j\in N_1} a_j z_j - \sum_{j\in N_2} a_j z_j > b, \\ & z \in B^n. \end{aligned}$$

Work in Progress...

- Is our problem NP-hard?
- Solving MILP:
  - Branch and Price Algorithm.
  - Benders decomposition.
  - Alternative approaches.
- Application to real data and comparison with typical classification methods.