



Semidefinite Programming: The Key to Semi-Supervised Support Vector Machines

Joint work with Veronica Piccialli* and Antonio M. Sudoso

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Support Vector Machines (SVMs) Vapnik & Chervonenkis (1963)

Input

- ▶ training set $\mathcal{T} = \{(x_i, y_i), i = 1, \dots, n, x_i \in \mathbb{R}^d, y_i \in \{-1, 1\}\}$



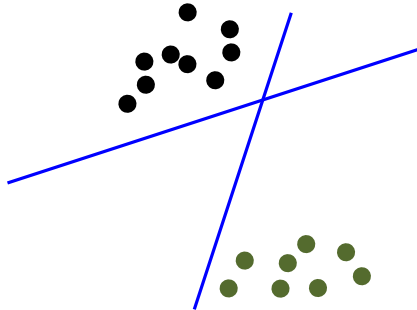
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Goal/Output

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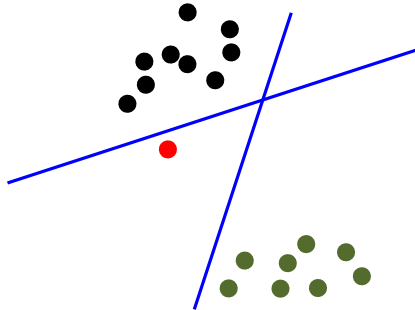
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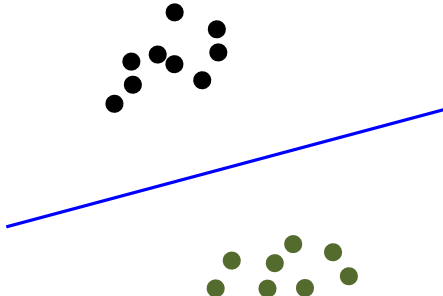
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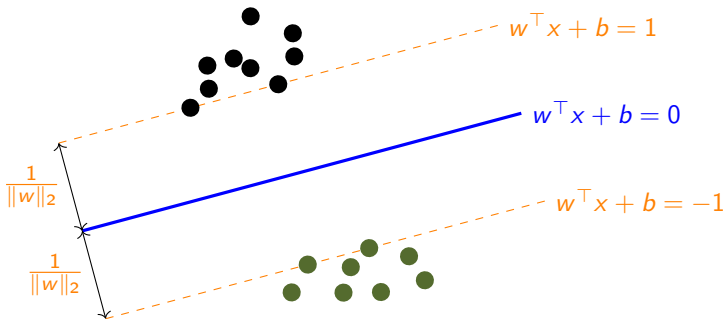
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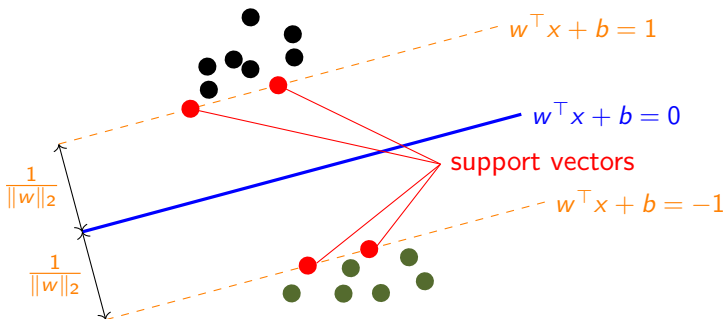
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Hard margin

Maximum hard margin hyperplane

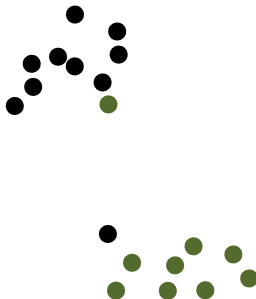
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Question: What if data is **not** linearly separable?



Soft margin Cortes & Vapnik (1995)

Maximum soft margin hyperplane w.r.t. $C > 0$

- ▶ data 'almost' linearly separable \Rightarrow allow **misclassifications**
- ▶ introduce slack variables ξ_i and add **penalty** term to objective:

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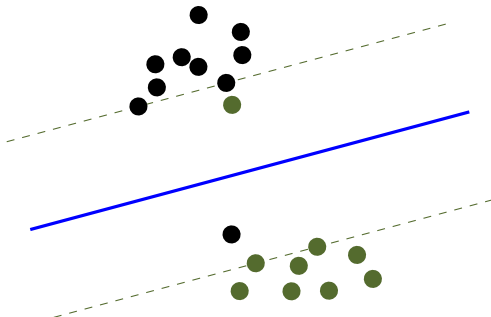
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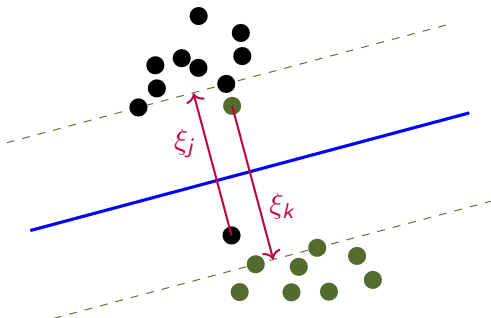
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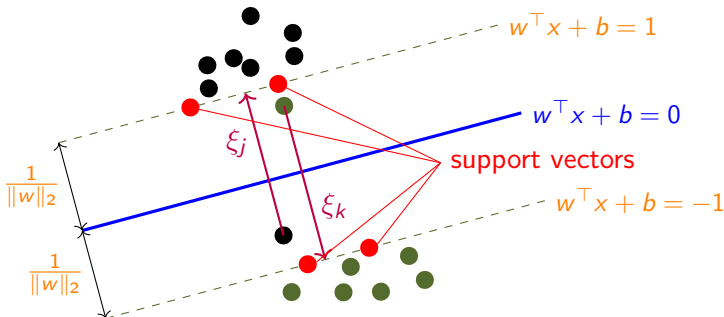
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Soft margin - dual problem

Wolfe dual

$$\begin{aligned} \min_{\alpha} \quad & \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n y_i y_j \langle x_i, x_j \rangle \alpha_i \alpha_j - \sum_{i=1}^n \alpha_i \\ \text{s. t.} \quad & \sum_{i=1}^n y_i \alpha_i = 0 \\ & 0 \leq \alpha_i \leq C, \quad i = 1, \dots, n \end{aligned}$$

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Let α^* be the optimal solution of the Wolfe dual. Then the maximum margin hyperplane (w^*, b^*) satisfies

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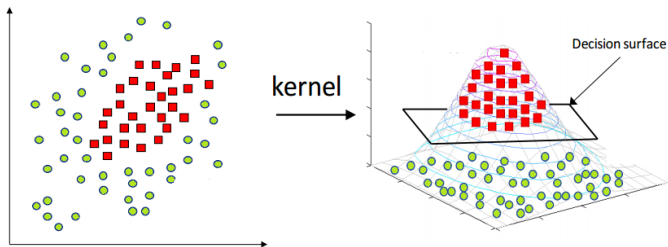
Decision function

$$y(x) = \text{sign} \left(\sum_{i=1}^n \alpha_i^* y_i \langle x_i, x \rangle + b^* \right).$$

Nonlinear SVMs: the kernel trick Boser, Guyon, Vapnik (1992)

Kernel trick

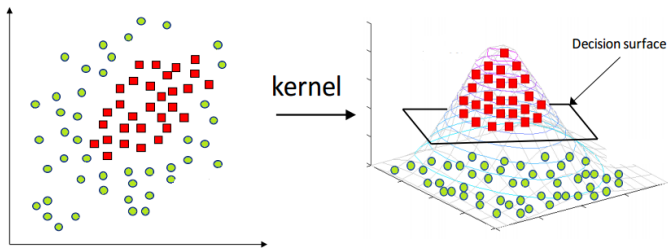
Map data into a **higher-dimensional** space via $\phi: \mathbb{R}^d \rightarrow \mathbb{R}^m, m \geq d$.
Then find a **separating hyperplane** in the new space.



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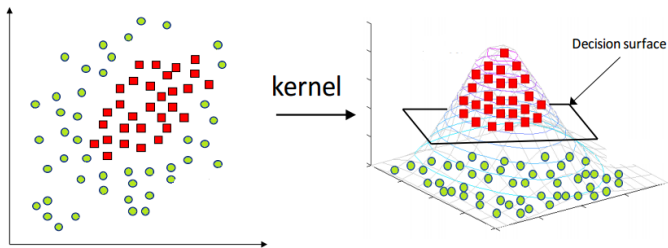
- ▶ linear or polynomial kernel, radial basis function kernel, ...
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$$k(x_i, x_j) := \langle \phi(x_i), \phi(x_j) \rangle$$

- ▶ separator is **nonlinear** in the original space

Kernel matrix

General kernel

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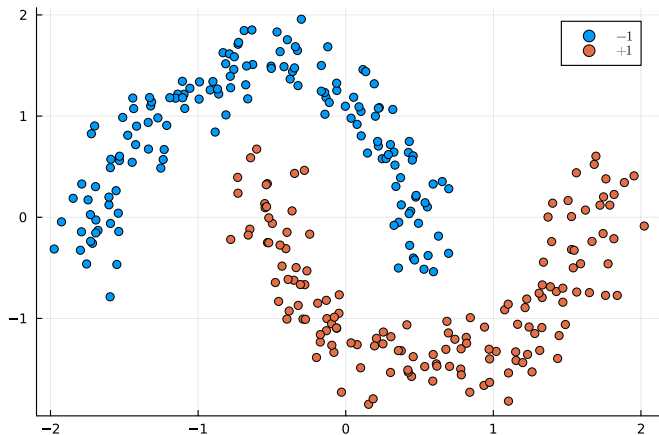
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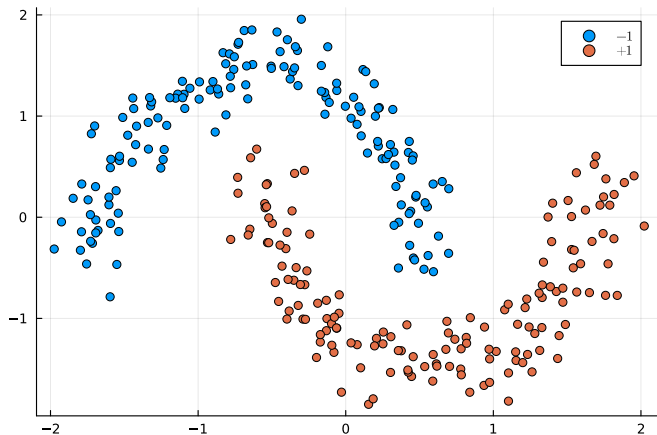
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Example: two moons dataset



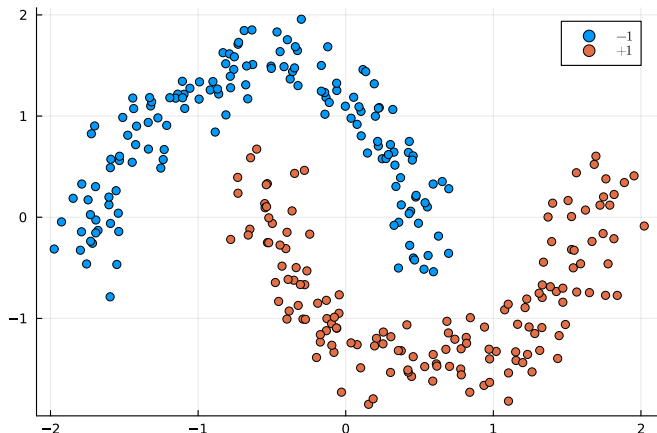
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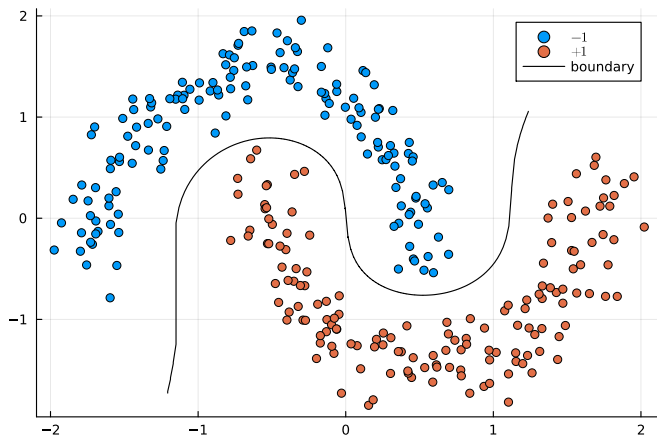
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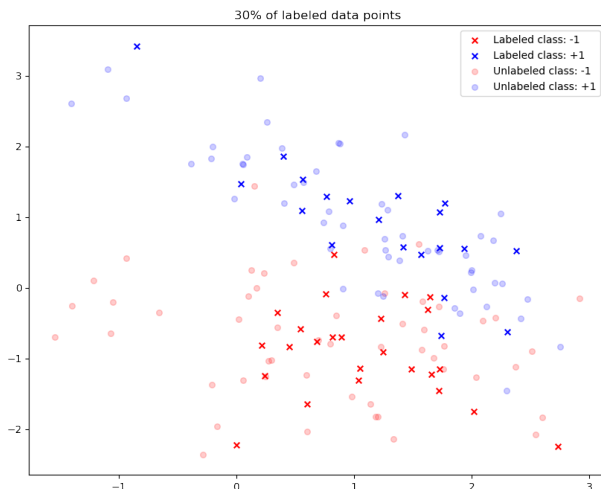
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Supervised learning

- ▶ **all** data must be labeled ...

Semi-supervised Support Vector Machines (S3VMs)

Bennett & Demiriz (1998)



► 70% of all labels are not known (and should be predicted)!

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Input

- ▶ n data points $x_i \in \mathbb{R}^d$, $i = 1, \dots, n$
- ▶ ℓ labeled points $\{(x_i, y_i)\}_{i=1}^{\ell}$ with $y_i \in \{-1, +1\}$, $i = 1, \dots, \ell$
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Kernel-based S3VM model

$$\begin{aligned} \min_{w, \xi, y^u} \quad & \frac{1}{2} \|w\|_2^2 + C_l \sum_{i=1}^{\ell} \xi_i^2 + C_u \sum_{i=\ell+1}^n \xi_i^2 \\ \text{s. t.} \quad & y_i w^\top \phi(x_i) \geq 1 - \xi_i, \quad i = 1, \dots, n \\ & y^u := (y_{\ell+1}, \dots, y_n) \in \{-1, +1\}^{n-\ell} \end{aligned}$$

When can semi-supervised learning work? Chapelle et al. (2006)

Semi-supervised smoothness assumption

If two points x_1, x_2 in a high-density region are close, then so should be the corresponding outputs y_1, y_2 .

Manifold assumption

The (high-dimensional) data lie (roughly) on a low-dimensional manifold.

Cluster assumption

If points are in the same cluster, they are likely to be of the same class.

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Low density separation

The decision boundary should lie in a low-density region.

Expectation vs. reality

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The S3VM performance increases with decreasing objective values.

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Bitter truth Chapelle et al. (2006, 2008)

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- ▶ often only the global optimum exhibits good performance
- ▶ **degenerate** local optima
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Goal: **exact** approach for S3VMs!

Reformulation of S3VM model with fewer variables

Notation

- ▶ kernel matrix $K^* \succeq 0$ with $K_{ij}^* = k(x_i, x_j) := \langle \phi(x_i), \phi(x_j) \rangle$
- ▶ diagonal matrix D with $D_{ii} = \begin{cases} \frac{1}{2C_l}, & \text{if } i \in \{1, \dots, \ell\} \\ \frac{1}{2C_u}, & \text{if } i \in \{\ell + 1, \dots, n\} \end{cases}$
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Reformulation as non-convex QCQP Bai & Yan (2016)

$$\begin{aligned} \min \quad & \frac{1}{2} v^\top K^{-1} v \\ \text{s. t.} \quad & y_i v_i \geq 1, \quad i = 1, \dots, \ell \\ & v_i^2 \geq 1, \quad i = \ell + 1, \dots, n \\ & v \in \mathbb{R}^n \end{aligned}$$

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- ▶ quadratic programming problem in **continuous** variables
- ▶ **convex** objective function
- ▶ **nonconvex** feasible set
- ▶ **bound constraints**: $y_i v_i \geq 1$ means either $v_i \leq -1$ or $v_i \geq 1$

Balancing constraint

Chapelle & Zien (2005): balancing constraint for linear kernel

$$\frac{1}{n - \ell} \sum_{i=\ell+1}^n \text{sign}(w^\top x_i) = \frac{1}{\ell} \sum_{i=1}^{\ell} y_i$$

- ▶ no degenerate solutions (all unlab. data points in one class)
- ▶ enhances performance and robustness

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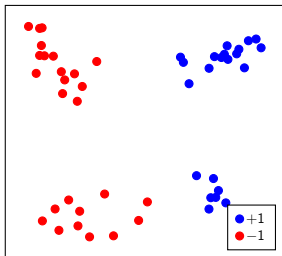
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We use the following “relaxation” instead:

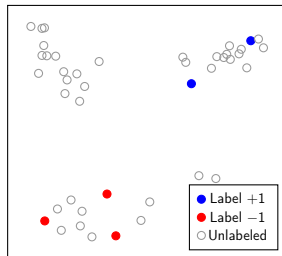
Soft-balancing constraint

$$\frac{1}{n - \ell} \sum_{i=\ell+1}^n v_i = \frac{1}{\ell} \sum_{i=1}^{\ell} y_i$$

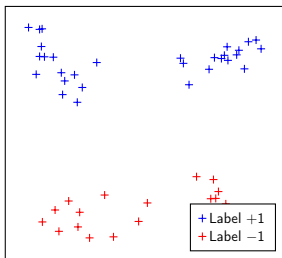
Illustration



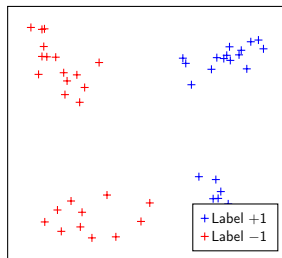
(a) ground-truth classification



(b) labeled and unlabeled data points



(c) optimal S3VM solution



(d) with balancing constraint

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Textbook-like form

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$$\mathbf{x} \in \mathbb{R}^n$$

► rename variables

Global optimization

Reformulation as non-convex QCQP Bai & Yan (2016)

$$\begin{array}{ll}\min & \frac{1}{2} v^T K^{-1} v \\ \text{s. t.} & y_i v_i \geq 1, \quad i = 1, \dots, \ell \\ & v_i^2 \geq 1, \quad i = \ell + 1, \dots, n \\ & v \in \mathbb{R}^n\end{array}$$

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- ▶ rename variables
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- ▶ some constraints redundant

Convex relaxations

Quadratic programming (QP) relaxation

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Bai & Yan (2016) introduce $X := xx^\top$ and relax to $X - xx^\top \succeq 0$:

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► Bai & Yan (2016): doubly nonnegative relaxation

Optimality-based box constraints

- ▶ feasible set **unbounded**
- ▶ IPM solvers like Mosek can **fail** to solve these SDPs **accurately**

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- ▶ UB: upper bound on optimal S3VM objective

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- ▶ any convex feasibility or optimality cut can be added
- ▶ (*) is equivalent to a convex **QP** with only **bound constraints**

SDP relaxation with bounded main diagonal

More stable SDP relaxation

$$\begin{aligned} \min \quad & \langle C, X \rangle \\ \text{s. t.} \quad & L_i \leq x_i \leq U_i, \quad i = 1, \dots, n \\ & 1 \leq X_{ii} \leq \max\{L_i^2, U_i^2\}, \quad i = 1, \dots, n \\ & \frac{1}{n-\ell} \sum_{i=\ell+1}^n x_i = \frac{1}{\ell} \sum_{i=1}^{\ell} y_i \\ & \bar{X} = \begin{pmatrix} 1 & x^\top \\ x & X \end{pmatrix} \succeq 0, \quad x \in \mathbb{R}^n, \quad X \in \mathcal{S}^n \end{aligned} \quad (*)$$

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For any feasible solution $\bar{X} \succeq 0$, we have:

$$\lambda_{\max}(\bar{X}) \leq \text{trace}(\bar{X}) \leq 1 + \sum_{i=1}^n \max\{L_i^2, U_i^2\}$$

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- ▶ solvers can exploit this information
- ▶ helps to find dual bounds on (*)

Reformulation Linearization Technique cuts Sherali & Adams (1998)

For any x_i, x_j , $i, j = 1, \dots, n$, we have:

$$\blacksquare U_i - x_i \geq 0$$

$$\blacksquare x_i - L_i \geq 0$$

$$\blacksquare U_j - x_j \geq 0$$

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$$\blacktriangleright (U_i - x_i)(x_j - L_j) \geq 0 \quad \Leftrightarrow \quad X_{ij} \leq U_i x_j + L_j x_i - U_i L_j$$

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RLT cuts

$$X_{ij} \geq \max\{U_i x_j + U_j x_i - U_i U_j, L_i x_j + L_j x_i - L_i L_j\},$$

$$X_{ij} \leq \min\{L_i x_j + U_j x_i - L_i U_j, U_i x_j + L_j x_i - U_i L_j\}.$$

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- \blacktriangleright cutting plane approach
- \blacktriangleright significant stronger lower bounds

Triangle inequalities Lambert (2023)

With three variables x_i, x_j, x_k :

$$(x_i - L_i)(x_j - L_j)(U_k - x_k) \geq 0$$

$$\Leftrightarrow$$

$$L_i L_j U_k - L_i L_j x_k - L_i U_k x_j + L_i x_j x_k - L_j U_k x_i + L_j x_i x_k + U_k x_i x_j \geq x_i x_j x_k$$

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Triangle cut

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- ▶ adding triangle cuts almost never improves lower bounds

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Balancing constraint

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- ▶ can be **linearized** in SDP relaxation
- ▶ **stronger** lower bounds but computation **slows down**

Optimality-based tightening Ryoo & Sahinidis (1995)

- ▶ UB: best known upper bound for **nonconvex** problem (P)
- ▶ LB: optimal value of SDP **relaxation**

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Optimality-based tightening (in our setting)

Let $g(x, X) \leq 0$ be an **active** constraint in the SDP relaxation with corresponding optimal dual multiplier $\lambda > 0$. Then the constraint

$$g(x, X) \geq -\frac{\text{UB} - \text{LB}}{\lambda}$$

is **valid** for all solutions of (P) with objective value **better than UB**.

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- ▶ $-\frac{\text{UB}-\text{LB}}{\lambda} \leq g(x, X) \leq 0$ for all optimal solutions (x, X) of (P)
- ▶ new constraint is **convex**

Bound tightening

If the constraint $L_i - x_i \leq 0$ is **active** at the optimal SDP solution with dual multiplier $\lambda_i^L > 0$, then the inequality

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$$(x, X) \text{ feasible for (P)} \Rightarrow 1 \leq x_i^2 = X_{ii} \leq \max\{L_i^2, U_i^2\}$$

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Lemma

Let $i \in \{1, \dots, n\}$. If the constraint $X_{ii} \geq 1$ is active at the optimal SDP solution with dual multiplier $\lambda > 0$, then we can update

$$L_i := \max \left\{ L_i, -\sqrt{1 + \frac{UB - LB}{\lambda}} \right\}, \quad U_i := \min \left\{ U_i, \sqrt{1 + \frac{UB - LB}{\lambda}} \right\}.$$

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Lemma

Let $i \in \{1, \dots, n\}$. Assume that a constraint of type $X_{ii} \leq \gamma$ is active at the optimal SDP solution with dual multiplier $\lambda > 0$ such that $p := \gamma - \frac{UB - LB}{\lambda} \geq 1$. Then the following holds:

- 1 If $L_i > -\sqrt{p}$, then we can update L_i via $L_i := \max\{L_i, \sqrt{p}\}$.
- 2 If $U_i < \sqrt{p}$, then we can update U_i via $U_i := \min\{U_i, -\sqrt{p}\}$.

Lower bound computation

- ① Find an initial good upper bound UB.
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Projecting box constraints

$$L_i > -1 \Rightarrow L_i := \max\{L_i, -1\} \quad \text{and} \quad U_i < 1 \Rightarrow U_i := \min\{U_i, 1\}$$

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Binary branching

- ▶ choose a variable x_i with $L_i \leq -1$ and $U_i \geq 1$
- ▶ set $U_i := -1$ in one subproblem and set $L_i := 1$ in the other

Primal heuristic

SVM with respect to $\bar{y} \in \{-1, 1\}^n$

$$\begin{aligned} \min \quad & x^\top Cx \\ \text{s. t.} \quad & \bar{y}_i x_i \geq 1, \quad i = 1, \dots, n, \\ & \frac{1}{n-\ell} \sum_{i=\ell+1}^n x_i = \frac{1}{\ell} \sum_{i=1}^{\ell} y_i, \\ & x \in \mathbb{R}^n \end{aligned} \tag{QP}$$

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Let (\hat{x}, \hat{X}) be the SDP solution.

- 1 Construct \bar{y} with entries $\bar{y}_i = \text{sign}(\hat{x}_i)$ and solve (QP).
- 2 Improve the solution found by applying a 2-opt local search with respect to the last $n - \ell$ entries of \bar{y} .

Computational results

- ▶ implementation in Julia using JuMP
- ▶ Mosek for SDPs and Gurobi for QPs
- ▶ optimality gap computed as $\varepsilon = \frac{UB-LB}{UB}$
- ▶ branch-and-bound is stopped when ε smaller than 0.1%
- ▶ results are averaged over three different seeds
- ▶ kernel and hyperparameters are chosen by 10-fold cross-validation

Root node relaxation for 10%, 20%, 30% labeled points

Instance	ℓ	$n - \ell$	Time Box [s]	Gap [%]	Time [s]	Iter
2moons	30	270	11.86	0.00	7.57	3.00
2moons	60	240	12.45	0.00	7.35	3.00
2moons	90	210	11.12	0.00	7.31	3.00
art150	14	136	1.30	0.04	1.44	3.00
art150	29	121	1.59	0.00	1.69	3.00
art150	44	106	1.32	0.01	1.38	3.00
connectionist	20	188	3.21	0.19	6.13	4.00
connectionist	41	167	3.09	0.16	9.84	4.67
connectionist	62	146	3.05	0.45	9.03	4.67
GunPoint	44	407	47.15	0.00	57.56	4.00
GunPoint	89	362	46.59	0.04	55.44	4.00
GunPoint	134	317	43.90	0.01	50.60	4.00
heart	27	243	6.92	0.22	10.36	4.00
heart	54	216	6.96	0.08	13.93	4.33
heart	81	189	6.37	0.15	12.05	4.33
ionosphere	34	317	19.84	0.66	19.53	3.67
ionosphere	70	281	19.67	0.01	20.73	3.33
ionosphere	104	247	17.98	0.00	27.77	4.00
PowerCons	36	324	21.80	0.04	22.79	3.67
PowerCons	72	288	19.12	0.01	26.26	4.00
PowerCons	108	252	18.87	0.01	28.53	4.00

Gurobi vs. SDP-S3VM

Instance	ℓ	$n - \ell$	Gurobi		SDP-S3VM		Solved
			Gap [%]	Time [s]	Gap [%]	Time [s]	
art100	10	90	7.37	3600	0.10	26.11	3
art100	20	80	3.09	2467.43	0.10	13.28	3
art100	30	70	3.27	2401.26	0.10	37.48	3
art150	14	136	8.44	3600	0.10	61.05	3
art150	29	121	2.72	1450.20	0.10	1.89	3
art150	44	106	2.52	2629.13	0.10	2.44	3
connectionist	20	188	16.83	3600	0.88	2587.20	1
connectionist	62	146	12.87	3600	0.10	248.07	3
connectionist	41	167	10.71	3600	0.10	104.95	3
heart	27	243	14.00	3600	0.10	38.89	3
heart	54	216	10.21	3600	0.10	64.45	3
heart	81	189	10.58	3600	0.10	16.22	3
2moons	30	270	6.52	3600	0.10	16.22	3
2moons	60	140	0.03	1023.52	0.10	22.07	3
2moons	90	210	0.05	1.95	0.10	21.50	3

► time limit of 3600 seconds

SVM vs. S3VM

Instance	ℓ	$n - \ell$	Kernel	Nodes	Time [s]	Acc. [%]	SVM [%]
ionosphere	34	317	RBF	59	529.48	91.80	81.70
ionosphere	34	317	linear	73	492.74	88.33	88.96
ionosphere	34	317	linear	3	50.05	87.38	84.23
ionosphere	70	281	RBF	3	107.89	90.75	90.04
ionosphere	70	281	RBF	7	181.61	91.46	85.05
ionosphere	70	281	linear	1	43.55	88.61	87.54
ionosphere	104	247	RBF	5	128.45	90.28	90.69
ionosphere	104	247	linear	37	221.45	88.26	86.64
ionosphere	104	247	linear	1	56.87	89.47	90.69
PowerCons	36	324	RBF	11	139.97	95.06	93.83
PowerCons	36	324	RBF	1	45.2	95.37	96.3
PowerCons	36	324	linear	53	534.19	97.84	94.44
PowerCons	72	288	RBF	11	101.41	95.83	94.79
PowerCons	72	288	RBF	1	30.79	96.53	97.57
PowerCons	72	288	linear	55	375.76	98.61	97.57
PowerCons	108	252	linear	11	129.53	98.81	98.81
PowerCons	108	252	linear	15	109.83	98.81	99.21
PowerCons	108	252	linear	17	169.85	98.41	99.21

Conclusion and future work

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- ▶ tools from global optimization essential
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Future work:

- ▶ first-order solver for SDPs
- ▶ parallel branch-and-bound

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Thank you!