An Exact Algorithm for Semi-Supervised Support Vector Machines using Strong SDP Bounds

April 17, 2024

Joint work with Veronica Piccialli* and Antonio M. Sudoso

*Veronica Piccialli's work has been supported by PNRR MUR project PE0000013-FAIR

FAIR Future Artificial Intelligence Research

FWF Der Wissenschaftsfonds.

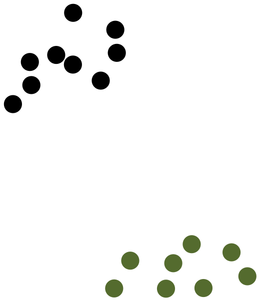
UNIVERSITÄT KLAGENFURT

Modeling - Analysis - Optimization DOC.FUNDS DOCTORAL SCHOOL

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

Input

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



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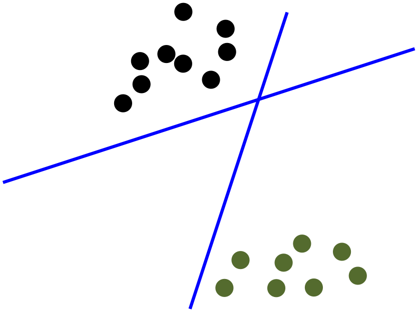
Goal/Output

- separating hyperplane $w^\top x + b = 0$



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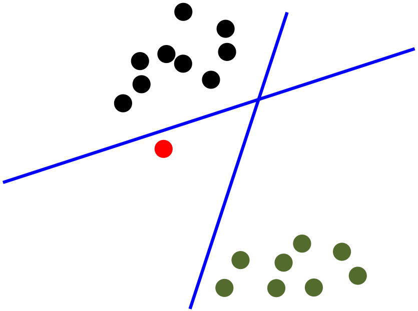
- separating hyperplane $w^\top x + b = 0$
- decision function $y(x) = \text{sign}(w^\top x + b)$ for new data



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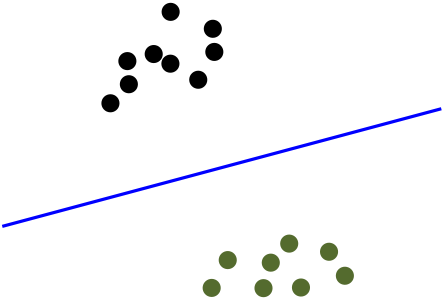

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- separating hyperplane $w^\top x + b = 0$ (maximum margin)
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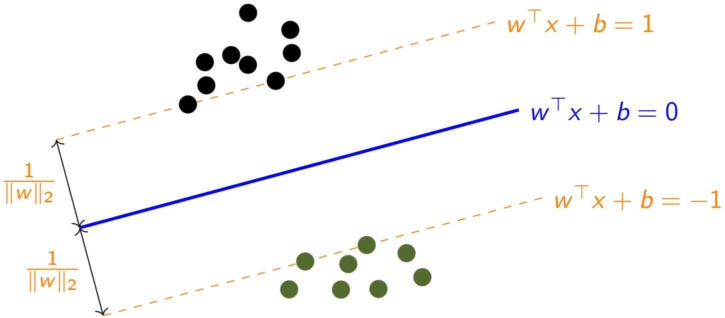

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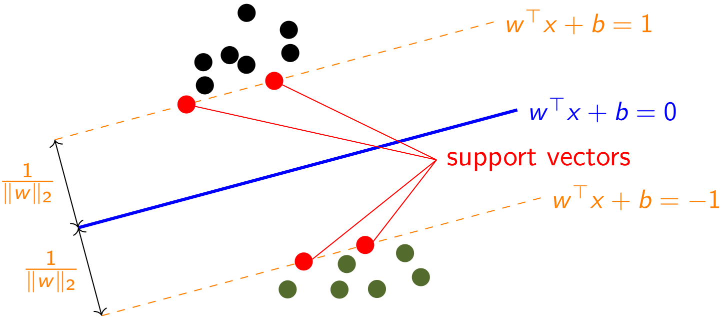

Hard margin

Maximum hard margin hyperplane

$$\begin{aligned} \min_{w,b} \quad & \tfrac{1}{2}\|w\|_2^2 \\ \text{s. t.} \quad & y_i[w^\top x_i + b] \geq 1, \; i = 1, \ldots, n \end{aligned}$$

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Maximum hard margin hyperplane

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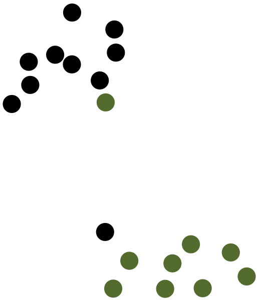
Question: What if the data is **not** linearly separable?



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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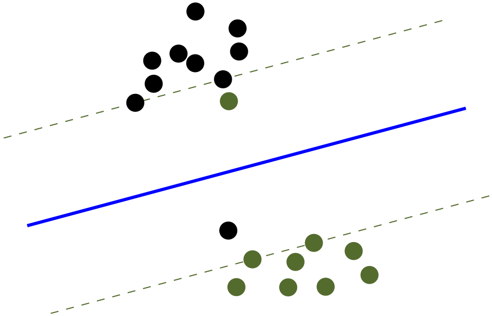

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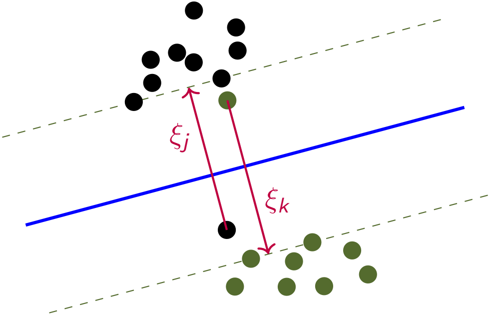

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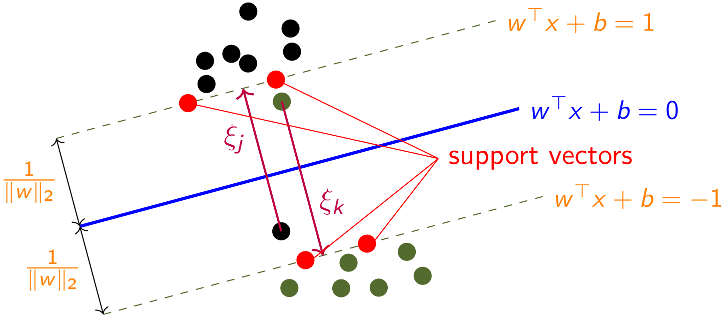

Soft margin - dual problem

Wolfe dual

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

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

$$w^* = \sum_{i=1}^{n} \alpha_i^* y_i x_i.$$

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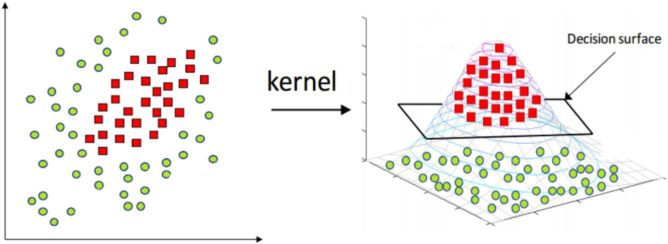
Decision function

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

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

Kernel trick

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



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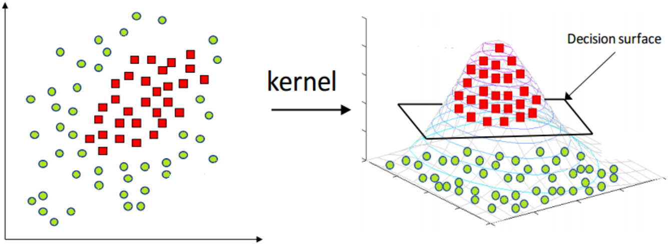

- linear or polynomial kernel, radial basis function kernel, ...
- no explicit mapping into higher dimension via kernel function

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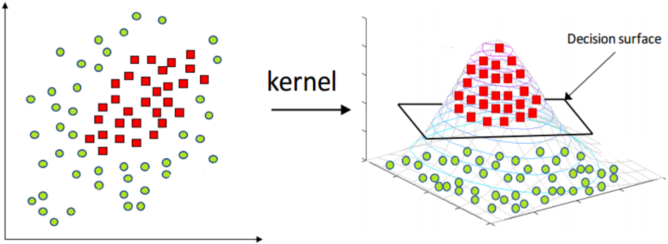

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- separator is nonlinear in the original space

Kernel matrix

General kernel

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

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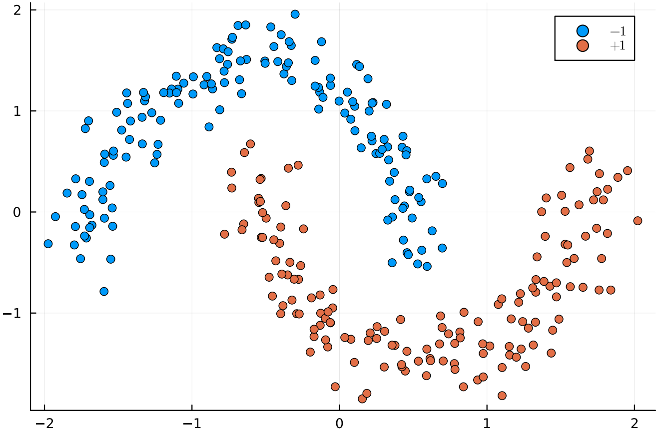
Example: two moons dataset



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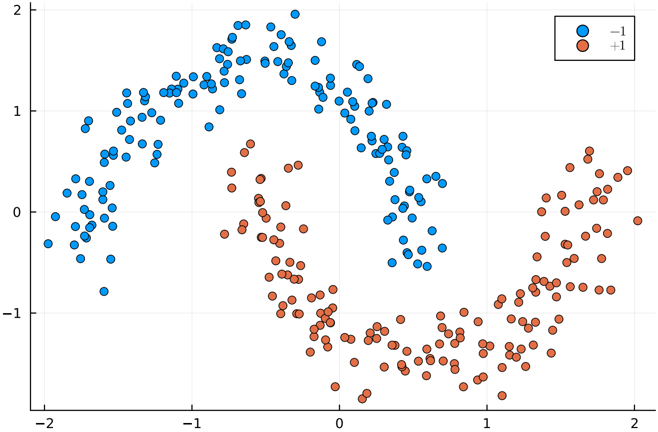

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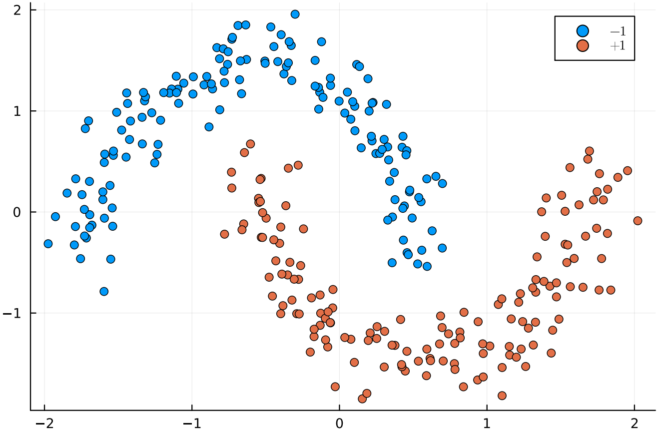

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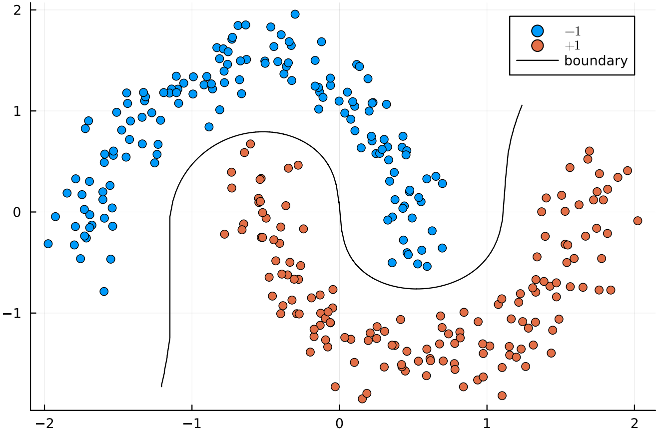

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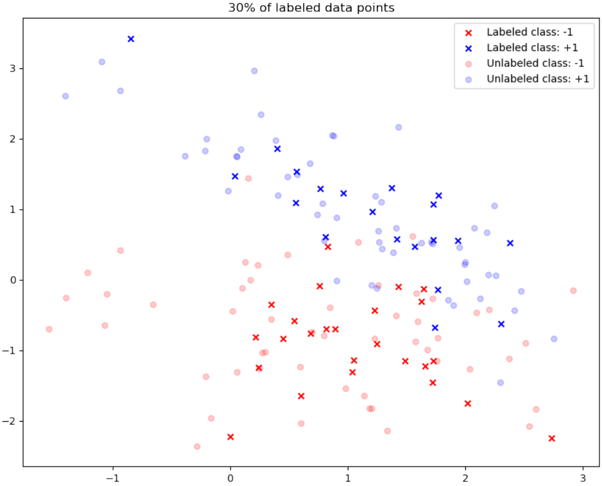
Supervised learning

- 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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- n data points $x_i \in \mathbb{R}^d, \ i = 1, \ldots, n$
- ℓ labeled points $\{(x_i, y_i)\}_{i=1}^{\ell}$ with $y_i \in \{-1, +1\}, \ i = 1, \ldots, \ell$
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Assumption

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Kernel-based S3VM model

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\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=l+1}^{n} \xi_i^2 \\
\text{s. t.} \quad & y_i\, w^\top \phi(x_i) \geq 1 - \xi_i,\ i = 1, \ldots, n \\
& y^u := (y_{\ell+1}, \ldots, 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

Expectation

The S3VM performance increases with decreasing objective values.

Expectation vs. reality

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The S3VM performance increases with decreasing objective values.

Bitter truth Chapelle et al. (2006, 2008)

- many local optima with poor performance
- often only the global optimum exhibits good performance
- degenerate local optima
- no heuristic method consistently finds the optimum

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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)

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\begin{aligned}
\min \quad & \tfrac{1}{2} v^\top K^{-1} v \\
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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

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

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

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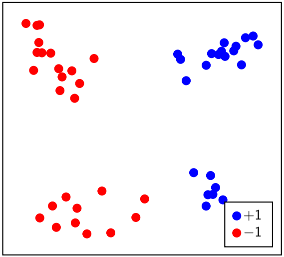
We use the following "relaxation" instead:

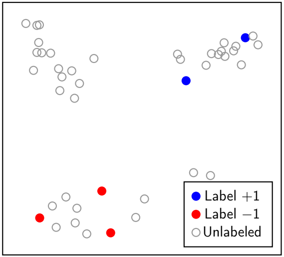
Soft-balancing constraint

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

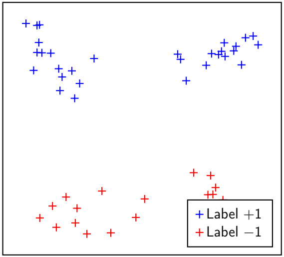
Illustration



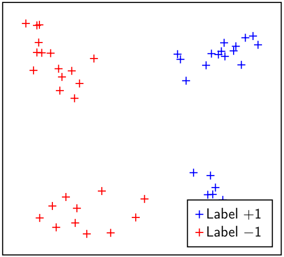
(a) ground-truth classification



(b) labeled and unlabeled data points



(c) optimal S3VM solution



(d) with balancing constraint

Global optimization

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Textbook-like form

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$$\begin{aligned} \min \quad & \\ \text{s. t.} \quad & \\ & \\ & x \in \mathbb{R}^n \end{aligned}$$

- rename variables

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$$\begin{aligned} \min \quad & x^\top C x \\ \text{s. t.} \quad & \\ & \\ & x \in \mathbb{R}^n \end{aligned}$$

- rename variables
- C symmetric and positive definite

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Textbook-like form

$$\begin{array}{ll} \min & x^\top C x \\ \text{s. t.} & L_i \leq x_i \leq U_i, \; i = 1, \dots, n \\ & \\ & x \in \mathbb{R}^n \end{array}$$

- rename variables
- C symmetric and positive definite
- $L_i \in \mathbb{R} \cup \{-\infty\}$ and $U_i \in \mathbb{R} \cup \{+\infty\}$

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- rename variables
- C symmetric and positive definite
- $L_i \in \mathbb{R} \cup \{-\infty\}$ and $U_i \in \mathbb{R} \cup \{+\infty\}$
- some constraints redundant

Quadratic programming (QP) relaxation

Textbook-like form

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\tag{QP}
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Matrix-based reformulation

We introduce $X := xx^\top$ and substitute $x_i x_j$ by X_{ij}:

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- $x^\top Cx = \langle C, xx^\top \rangle = \langle C, X \rangle$
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- $X \succeq 0$
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Semidefinite programming (SDP) relaxation

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LP and SDP: conic programs

LP

$$\begin{aligned} \min \quad & c^\top x \\ \text{s. t.} \quad & Ax = b \\ & x \in \mathbb{R}^n_+ \quad (x \geq 0) \end{aligned}$$

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- $\mathcal{S}^n_+$: cone of positive semidefinite matrices

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- $\mathcal{S}^n_+$: cone of positive semidefinite matrices
- every LP can be rewritten as an of polynomial size SDP
- well-posed SDPs can be solved in polynomial time
- duality theory for SDPs

Optimality-based box constraints

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

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Convex QCQP

$$\begin{aligned} L_i / U_i := \min / \max \quad & x_i \\ \text{s.t.} \quad & L_i \leq x_i \leq U_i, \; i = 1, \ldots, n \\ & x^\top C x \leq \text{UB} \\ & x \in \mathbb{R}^n \end{aligned} \tag{$*$}$$

- UB: upper bound on optimal S3VM objective

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\end{aligned} \tag{$*$}
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- UB: upper bound on optimal S3VM objective
- we could also solve SDPs instead
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- we could also solve SDPs instead
- any convex feasibility or optimality cut can be added
- $(*)$ is equivalent to a convex QP with only bound constraints

Solving the dual problem

Computing U_i

$$\begin{aligned} \max \quad & x_i \\ \text{s. t.} \quad & L_j \le x_j \le U_j, \quad j = 1, \dots, n, \\ & x^\top C x \le \mathrm{UB} \end{aligned} \tag{$*$}$$

Prerequisite

We set $U_i := \infty$ in $(*)$.

Solving the dual problem

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We set $U_i := \infty$ in $(*)$.

Dual problem

$$\begin{aligned} \min \quad & \frac{1}{4\mu} \left(e_i + \lambda^L - \lambda^U\right)^\top C^{-1} \left(e_i + \lambda^L - \lambda^U\right) - L^\top \lambda^L + U^\top \lambda^U + \mu \mathrm{UB} \\ \text{s.t.} \quad & \lambda^L, \lambda^U \ge 0, \; \mu > 0. \end{aligned}$$

Solving the dual problem

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- only bound constraints
- objective function is differentiable $\hookrightarrow$ use L-BFGS-B

SDP relaxation with bounded main diagonal

More stable SDP relaxation

$$
\begin{aligned}
\min \quad & \langle C, X\rangle \\
\text{s.t.} \quad & L_i \le x_i \le U_i,\ i = 1, \dots, n \\
& 1 \le X_{ii} \le \max\{L_i^2, U_i^2\},\ i = 1, \dots, n \qquad (*) \\
& \bar{X} = \begin{pmatrix} 1 & x^\top \\ x & X \end{pmatrix} \succeq 0,\ x \in \mathbb{R}^n,\ X \in \mathcal{S}^n
\end{aligned}
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For any feasible solution $\bar{X} \succeq 0$, we have:

$$
\lambda_{\max}(\bar{X}) \le \operatorname{trace}(\bar{X}) \le 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 $x_i, x_j,\ i, j = 1, \ldots, n$, we have:

- $U_i - x_i \geq 0$
- $x_i - L_i \geq 0$

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

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

- cutting plane approach
- 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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$$(U_i - x_i)(U_j - x_j)(x_k - L_k) \geq 0$$
$$\Leftrightarrow$$
$$x_i x_j x_k \geq L_k U_i U_j + L_k x_i x_j - U_i U_j x_k + U_j x_i x_k + U_i x_j x_k - L_k U_j x_i - L_k U_i x_j$$

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$$(U_i - x_i)(U_j - x_j)(x_k - L_k) \geq 0$$
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Triangle cut

$$\begin{aligned}(U_k - L_k)x_i x_j + (L_j - U_j)x_i x_k + (L_i - U_i)x_j x_k + L_i L_j U_k - L_k U_i U_j \\ + (L_k U_j - L_j U_k)x_i + (L_k U_i - L_i U_k)x_j + (U_i U_j - L_i L_j)x_k \geq 0\end{aligned}$$

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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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- adding triangle cuts almost never improves lower bounds

Product constraints

Balancing constraint

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

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Product constraints

$$\frac{1}{n-\ell}\sum_{i=\ell+1}^{n} x_i x_j = \Big(\frac{1}{\ell}\sum_{i=1}^{\ell} y_i\Big) x_j, \quad j = 1, \ldots, n$$

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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)
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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

Marginals-based bound tightening Ryoo & Sahinidis (1995)

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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can be added to (P) and to the SDP relaxation.

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- if $\lambda_i^L > 0$, update U_i via $U_i := \min\left\{U_i, L_i + \frac{\mathrm{UB}-\mathrm{LB}}{\lambda_i^L}\right\}$

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can be added to (P) and to the SDP relaxation.

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- if $\lambda_i^U > 0$, update L_i via $L_i := \max\left\{L_i, U_i - \frac{\text{UB}-\text{LB}}{\lambda_i^U}\right\}$

Applying optimality-based tightening to main diagonal

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

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

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Lemma

Let $i \in \{1, \ldots, n\}$. 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 $U_i := \min\{U_i, -\sqrt{p}\}$.*

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1. Find an initial good upper bound UB.
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$L_i > -1 \;\Rightarrow\; L_i := \max\{L_i, 1\}$ and $U_i < 1 \;\Rightarrow\; U_i := \min\{U_i, -1\}$

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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 $\bar{y} \in \{-1, 1\}^n$

$$\begin{aligned} \min \quad & x^\top C x \\ \text{s.t.} \quad & \bar{y}_i x_i \geq 1, \; i = 1, \ldots, n, \\ & x \in \mathbb{R}^n \end{aligned} \tag{QP}$$

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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 2-opt local search.

Computational results

- implementation in `Julia` using `JuMP`
- `Mosek` for SDPs and `Gurobi` for QPs
- optimality gap computed as $\varepsilon = \frac{\text{UB}-\text{LB}}{\text{UB}}$
- 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 Gap [%]	Gurobi Time [s]	SDP-S3VM Gap [%]	SDP-S3VM Time [s]	SDP-S3VM Solved
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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- S3VM models can be solved to optimality
- tools from global optimization essential
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Thank you!