A novel embedded min-max approach for feature selection in nonlinear Support Vector Machine classification

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June 10th, 2021

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Outline

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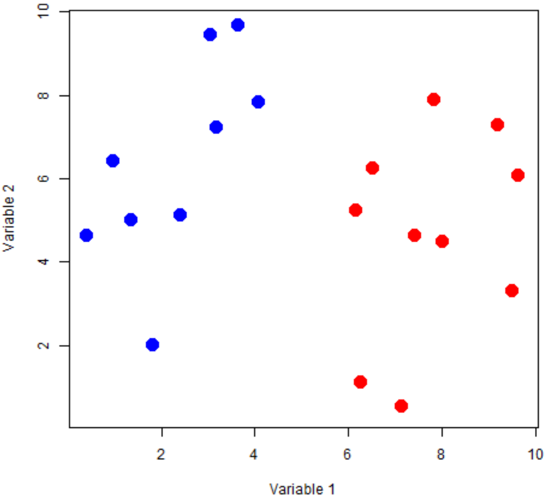
Binary Classification Problem.



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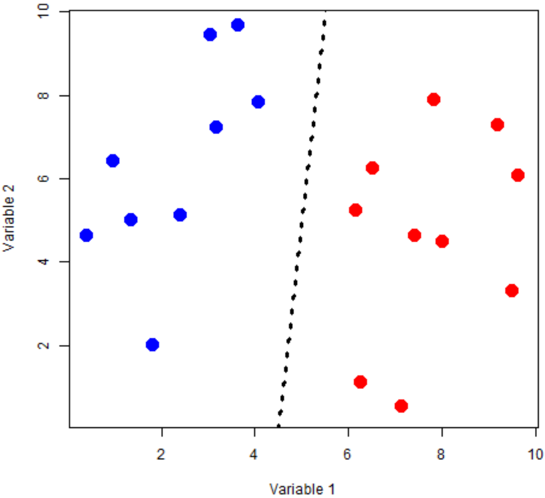

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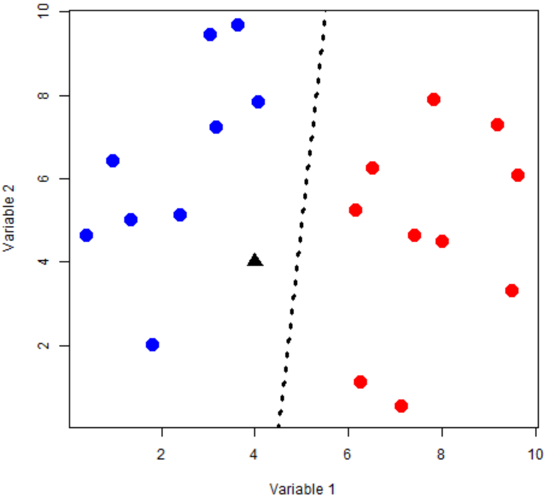

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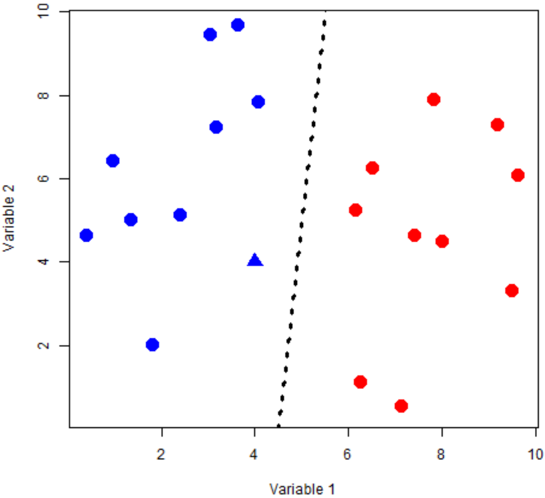
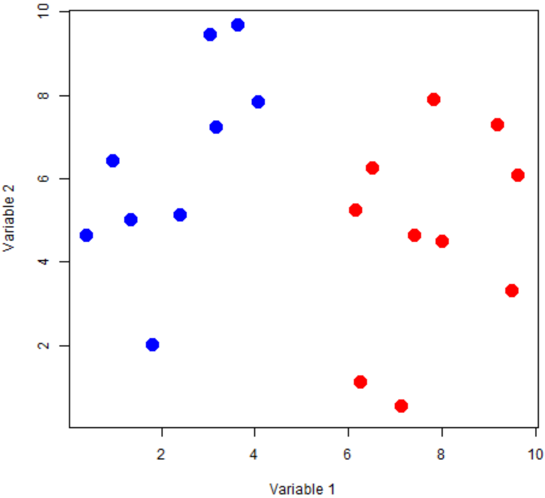


Binary Classification Problem. Feature Selection



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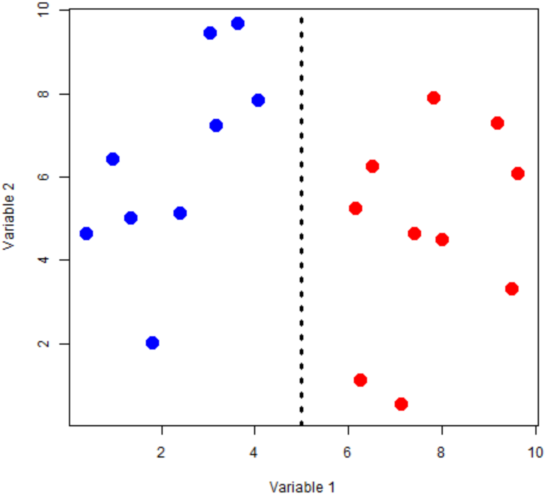
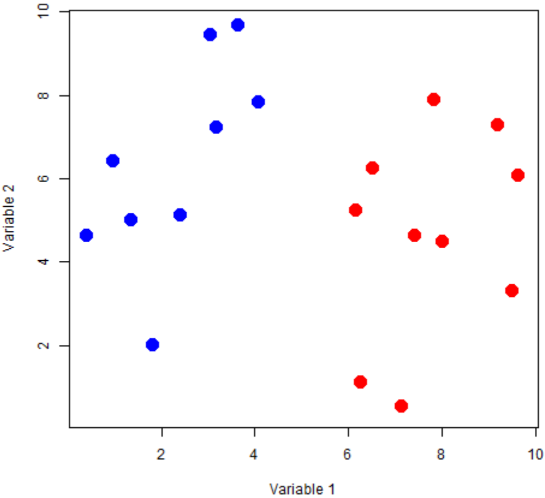


Support Vector Machines (SVM)



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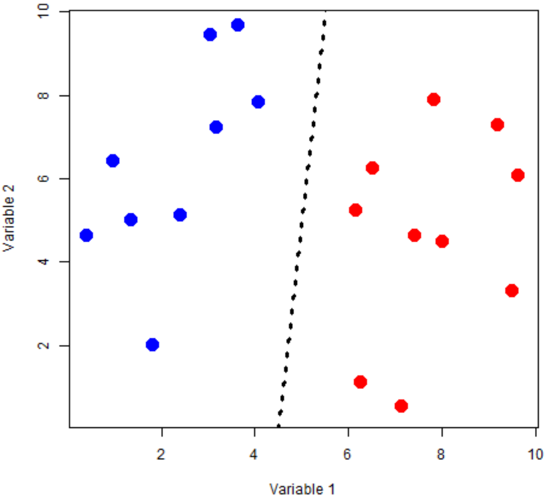

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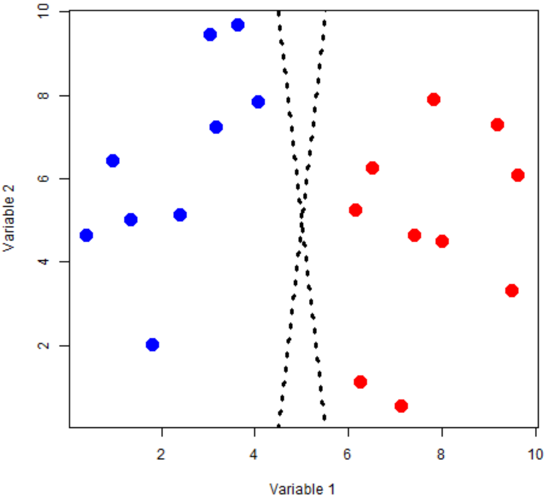

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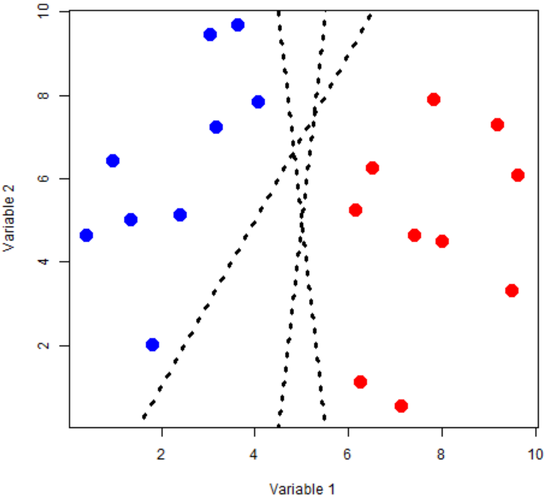

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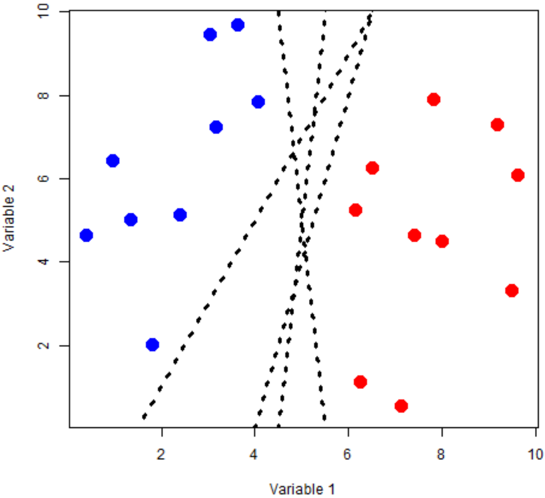

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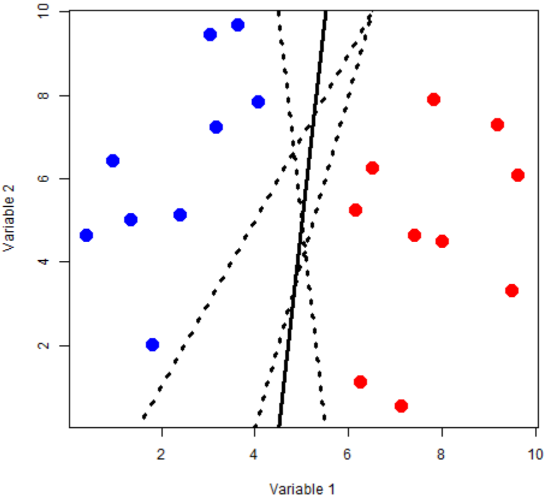

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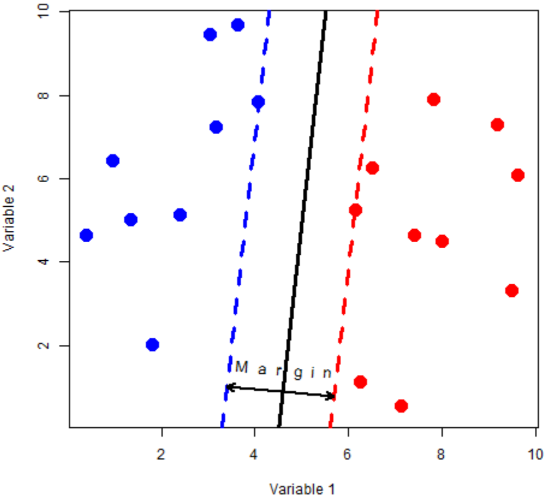

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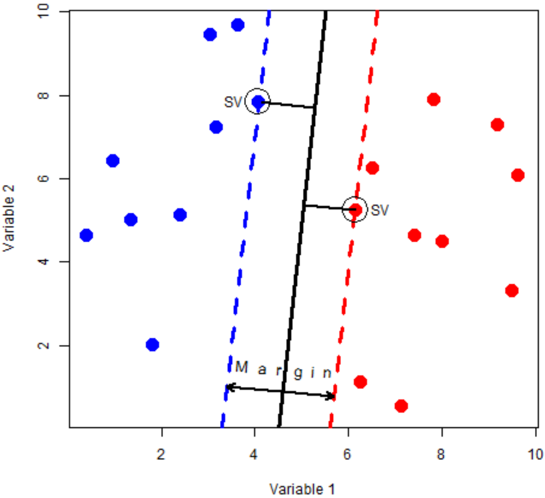
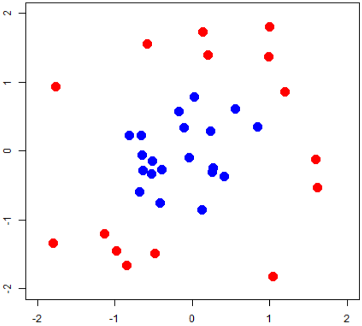


What happens in the nonlinear case?



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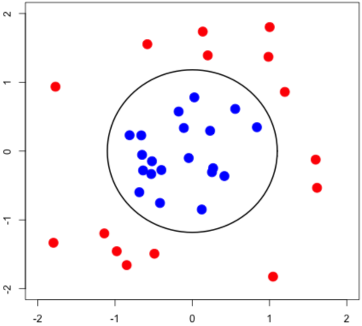

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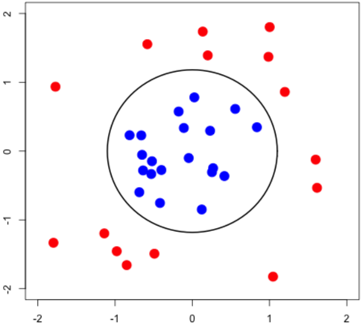
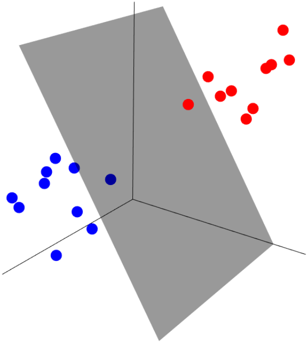


$$\overset{\phi}{\Longrightarrow}$$



Aim

- Develop a new Mathematical Optimization approach to perform feature selection in a binary classification problem.
- Classification tool: Support Vector Machine (SVM).
- Min-max approach.

Literature Review

- Linear: *Gaudioso et al. [2017]; Labbé et al. [2019]; Maldonado et al. [2014]*; ...

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- **Nonlinear:**
  - Filter (kernel polarization, *Wang et al. [2010]*):
    - Most separated classes in high-dimensional space.
    - Fast, but not take into account classifier information.

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- **Nonlinear:**
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  - Wrapper

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- **Nonlinear:**
  - Filter (kernel polarization, *Wang et al. [2010]*):
  - Wrapper (min-max RFE, *Onel et al. [2019]*):
    - Min-max approach with binary variables.
    - Fixed # of selected features.
    - Equivalent RFE-SVM which sequentially removes features.

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- **Nonlinear:**
  - Filter (kernel polarization, *Wang et al. [2010]*):
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  - Embedded

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  - Embedded (KP-SVM, *Maldonado et al. [2011]*):
    - ℓ_0-(pseudo)norm approximation to dual SVM.
    - Large number of hyperparameters.
    - Ad-hoc approaches.

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Our contributions

- Embedded feature selection method.
- # selected features is not fixed, but provided by our methodology.
- No ad-hoc strategies. Off-the-shelf solvers.

Outline

SVM Problem (Primal).

Data: $x_i \in \mathbb{R}^M$ Class label: $y_i \in \{-1, 1\}$

$$\left\{ \begin{array}{rl} \min\limits_{w,\,b,\,\xi} & \frac{1}{2}\|w\|^2 + C \sum\limits_{i \in \mathcal{S}} \xi_i \\ \text{s.t.} & (w' \quad x_i \ + b) y_i \geq 1 - \xi_i, \quad i \in \mathcal{S} \\ & \xi_i \geq 0, \quad i \in \mathcal{S} \end{array} \right.$$

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SVM Problem (Primal).

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Unfortunately

ϕ and $\mathcal{F}_\gamma$ are usually unknown.

SVM Problem (Dual). Feature Selection.

Data: $x_i \in \mathbb{R}^M$ Class label: $y_i \in \{-1, 1\}$

$$\left\{ \begin{array}{rl} \min\limits_{\gamma} \max\limits_{\boldsymbol{\alpha}} & \sum\limits_{i \in \mathcal{S}} \alpha_i - \frac{1}{2} \sum\limits_{i,\ell \in \mathcal{S}} \alpha_i \alpha_\ell y_i y_\ell \phi(x_i)' \phi(x_\ell) \\ \text{s.t.} & \sum\limits_{i \in \mathcal{S}} \alpha_i y_i = 0 \\ & \alpha_i \in [0, C], \quad i \in \mathcal{S} \end{array} \right.$$

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\end{array}
\right.
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Kernel trick

$$K_\gamma(x_i, x_\ell) = \phi(x_i)' \phi(x_\ell)$$

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SVM Problem. Kernel.

Anisotropic Gaussian kernel

$$K_\gamma(x_i, x_\ell) = \exp\left(-\sum_{j=1}^{M} \boldsymbol{\gamma_j}(x_{ij} - x_{\ell j})^2\right)$$

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γ_j: importance feature j

- $\gamma_j \to 0$: no role in the classification.
- large γ_j: critical when classifying.

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Trade-off

- Model complexity.
- Classification accuracy.

Problem Formulation

$$
\begin{cases}
\min\limits_{\gamma \geq 0} \left[\max\limits_{\boldsymbol{\alpha}} \sum\limits_{i \in \mathcal{S}} \alpha_i - \frac{1}{2} \sum\limits_{i,\ell \in \mathcal{S}} \alpha_i \alpha_\ell y_i y_\ell K_\gamma(x_i, x_\ell) \right] \\
\text{s.t.} \sum\limits_{i \in \mathcal{S}} \alpha_i y_i = 0 \\
0 \leq \alpha_i \leq C, \forall i
\end{cases}
$$

Classification accuracy

Problem Formulation

$$\begin{cases} \min\limits_{\gamma \geq 0} \left[\quad \|\gamma\|_p^p + \qquad \begin{array}{l} \max\limits_{\alpha} \sum\limits_{i \in \mathcal{S}} \alpha_i - \frac{1}{2} \sum\limits_{i,\ell \in \mathcal{S}} \alpha_i \alpha_\ell y_i y_\ell K_\gamma(x_i, x_\ell) \end{array} \right] \\ \qquad\qquad\qquad\qquad \text{s.t.} \sum\limits_{i \in \mathcal{S}} \alpha_i y_i = 0 \\ \qquad\qquad\qquad\qquad\qquad 0 \leq \alpha_i \leq C, \forall i \end{cases}$$

Model complexity

Classification accuracy

Problem Formulation

$$\begin{cases} \min\limits_{\gamma \geq 0} \left[C_2 \|\gamma\|_p^p + (1 - C_2) \max\limits_{\alpha} \sum\limits_{i \in \mathcal{S}} \alpha_i - \frac{1}{2} \sum\limits_{i,\ell \in \mathcal{S}} \alpha_i \alpha_\ell y_i y_\ell K_\gamma(x_i, x_\ell) \right] \\ \qquad \text{s.t.} \sum\limits_{i \in \mathcal{S}} \alpha_i y_i = 0 \\ \qquad 0 \leq \alpha_i \leq C, \forall i \end{cases}$$

Model complexity

Classification accuracy

Trade-off

Outline

Min-max optimization problem.

$$\begin{cases} \min\limits_{\gamma \geq 0} \left[C_2 \|\gamma\|_p^p + (1 - C_2) \max\limits_{\alpha} \sum\limits_{i \in \mathcal{S}} \alpha_i - \frac{1}{2} \sum\limits_{i,\ell \in \mathcal{S}} \alpha_i \alpha_\ell y_i y_\ell K_\gamma(x_i, x_\ell) \right] \\ \qquad\qquad\qquad\qquad \text{s.t.} \quad \sum\limits_{i \in \mathcal{S}} \alpha_i y_i = 0 \\ \qquad\qquad\qquad\qquad\qquad 0 \leq \alpha_i \leq C, \forall i \end{cases}$$

Epigraph form.

$$
\begin{cases}
\min\limits_{\gamma \geq 0,\, \boldsymbol{z}} \; C_2 \|\gamma\|_p^p + (1 - C_2)\boldsymbol{z} \\[2ex]
\text{s.t.} \quad \boldsymbol{z \geq \max\limits_{\alpha} \sum_{i \in \mathcal{S}} \alpha_i - \frac{1}{2} \sum_{i, \ell \in \mathcal{S}} \alpha_i \alpha_\ell y_i y_\ell K_\gamma(x_i, x_\ell)} \\[2ex]
\qquad\qquad\qquad\quad \textbf{s.t.} \; \boldsymbol{\sum_{i \in \mathcal{S}} \alpha_i y_i = 0} \\[2ex]
\qquad\qquad\qquad\qquad \boldsymbol{0 \leq \alpha_i \leq C,\, \forall i}
\end{cases}
$$

Strong duality lower level problem (SVM).

$$
\begin{cases}
\min\limits_{\gamma \geq 0, z} \; C_2 \|\gamma\|_p^p + (1 - C_2) z \\
\text{s.t.} \quad z \geq \max\limits_{\alpha} \sum\limits_{i \in \mathcal{S}} \alpha_i - \dfrac{1}{2} \sum\limits_{i, \ell \in \mathcal{S}} \alpha_i \alpha_\ell y_i y_\ell K_\gamma(x_i, x_\ell) \\
\qquad\qquad \text{s.t.} \; \sum\limits_{i \in \mathcal{S}} \alpha_i y_i = 0 & \boldsymbol{(\nu)} \\
\qquad\qquad\qquad 0 \leq \alpha_i \leq C, \, \forall i & \boldsymbol{(\lambda_i^0, \lambda_i^C)}
\end{cases}
$$

Strong duality lower level problem (SVM).

Dual lower-level problem. Lagrangian. $[G_\gamma = diag(y) K_\gamma diag(y)]$

$$\begin{cases} \min\limits_{\alpha,\nu,\lambda^0,\lambda^C} & -\dfrac{1}{2}\alpha' G_\gamma \alpha + (e - \nu y + \lambda^0 - \lambda^C)'\alpha + C(\lambda^C)'e \\ \text{s.t.} & G_\gamma \alpha - (e - \nu y + \lambda^0 - \lambda^C) = 0 \\ & \lambda^0, \lambda^C \geq 0 \\ & 0 \leq \alpha \leq C \end{cases}$$

Strong duality lower level problem (SVM).

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\qquad\qquad \text{s.t.} \quad \sum\limits_{i \in \mathcal{S}} \alpha_i y_i = 0 \\
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\end{cases}
$$

Dual lower-level problem. Lagrangian. $[G_\gamma = diag(y) K_\gamma diag(y)]$

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\begin{cases}
\min\limits_{\alpha, \nu, \lambda^0, \lambda^C} \; -\dfrac{1}{2} \alpha' G_\gamma \alpha + (e - \nu y + \lambda^0 - \lambda^C)' \alpha + C (\lambda^C)' e \\
\quad \text{s.t.} \quad G_\gamma \alpha - (e - \nu y + \lambda^0 - \lambda^C) = 0 \\
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\end{cases}
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Strong duality lower level problem (SVM).

$$
\begin{cases}
\min\limits_{\gamma \geq 0,\, z} \; C_2 \|\gamma\|_p^p + (1 - C_2) z \\
\text{s.t.} \quad z \geq \min\limits_{\boldsymbol{\alpha}, \boldsymbol{\nu}, \boldsymbol{\lambda}^{\mathbf{0}}, \boldsymbol{\lambda}^{\boldsymbol{C}}} \; -\frac{1}{2} \boldsymbol{\alpha}' \boldsymbol{G}_{\boldsymbol{\gamma}} \boldsymbol{\alpha} + (\boldsymbol{e} - \boldsymbol{\nu} \boldsymbol{y} + \boldsymbol{\lambda}^{\mathbf{0}} - \boldsymbol{\lambda}^{\boldsymbol{C}})' \boldsymbol{\alpha} + \boldsymbol{C} (\boldsymbol{\lambda}^{\boldsymbol{C}})' \boldsymbol{e} \\
\qquad\qquad \textbf{s.t.} \quad \boldsymbol{G}_{\boldsymbol{\gamma}} \boldsymbol{\alpha} - (\boldsymbol{e} - \boldsymbol{\nu} \boldsymbol{y} + \boldsymbol{\lambda}^{\mathbf{0}} - \boldsymbol{\lambda}^{\boldsymbol{C}}) = \mathbf{0} \\
\qquad\qquad\qquad \boldsymbol{\lambda}^{\mathbf{0}}, \boldsymbol{\lambda}^{\boldsymbol{C}} \geq \mathbf{0} \\
\qquad\qquad\qquad \mathbf{0} \leq \boldsymbol{\alpha} \leq \boldsymbol{C}
\end{cases}
$$

Dual lower-level problem. Lagrangian. $[G_\gamma = diag(y) K_\gamma diag(y)]$

$$
\begin{cases}
\min\limits_{\alpha, \nu, \lambda^0, \lambda^C} \; -\frac{1}{2} \alpha' G_\gamma \alpha + (e - \nu y + \lambda^0 - \lambda^C)' \alpha + C (\lambda^C)' e \\
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\qquad\qquad \lambda^0, \lambda^C \geq 0 \\
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\end{cases}
$$

Single-level optimization problem

$$\begin{cases} \min\limits_{\gamma,\,\alpha,\nu,\lambda^0,\lambda^C} C_2\|\gamma\|_p^p - (1-C_2)\left(\frac{1}{2}\alpha' G_\gamma \alpha - (e-\nu y+\lambda^0-\lambda^C)'\alpha - C(\lambda^C)'e\right) \\ \quad\text{s.t.}\ \ G_\gamma\alpha - (e-\nu y+\lambda^0-\lambda^C) = 0 \\ \qquad\quad \gamma,\lambda^0,\lambda^C \geq 0 \\ \qquad\quad 0 \leq \alpha \leq C \end{cases}$$

Recap

$$\min_{\gamma \geq 0} \left[C_2 \|\gamma\|_p^p + (1 - C_2) \max_{\alpha} \sum_{i \in \mathcal{S}} \alpha_i - \frac{1}{2} \sum_{i,\ell \in \mathcal{S}} \alpha_i \alpha_\ell y_i y_\ell K_\gamma(x_i, x_\ell) \right]$$

$$\text{s.t.} \sum_{i \in \mathcal{S}} \alpha_i y_i = 0$$

$$0 \leq \alpha_i \leq C, \forall i$$

Recap

$$\min_{\gamma \geq 0} \left[C_2 \|\gamma\|_p^p + (1 - C_2) \max_{\alpha} \sum_{i \in \mathcal{S}} \alpha_i - \frac{1}{2} \sum_{i,\ell \in \mathcal{S}} \alpha_i \alpha_\ell y_i y_\ell K_\gamma(x_i, x_\ell) \right]$$

$$\text{s.t.} \quad \sum_{i \in \mathcal{S}} \alpha_i y_i = 0$$

$$0 \leq \alpha_i \leq C, \forall i$$

$$\min_{\gamma \geq 0, z} C_2 \|\gamma\|_p^p + (1 - C_2) z$$

$$\text{s.t.} \quad z \geq \max_{\alpha} \sum_{i \in \mathcal{S}} \alpha_i - \frac{1}{2} \sum_{i,\ell \in \mathcal{S}} \alpha_i \alpha_\ell y_i y_\ell K_\gamma(x_i, x_\ell)$$

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$$0 \leq \alpha_i \leq C, \forall i$$

Recap

$$\min_{\gamma\geq 0}\left[C_2\|\gamma\|_p^p+(1-C_2)\max_{\alpha}\sum_{i\in\mathcal{S}}\alpha_i-\frac{1}{2}\sum_{i,\ell\in\mathcal{S}}\alpha_i\alpha_\ell y_i y_\ell K_\gamma(x_i,x_\ell)\right]$$
$$\text{s.t.}\quad \sum_{i\in\mathcal{S}}\alpha_i y_i=0$$
$$0\leq\alpha_i\leq C,\forall i$$

$$\min_{\gamma\geq 0,z} C_2\|\gamma\|_p^p+(1-C_2)z$$
$$\text{s.t.}\quad z\geq\max_{\alpha}\sum_{i\in\mathcal{S}}\alpha_i-\frac{1}{2}\sum_{i,\ell\in\mathcal{S}}\alpha_i\alpha_\ell y_i y_\ell K_\gamma(x_i,x_\ell)$$
$$\text{s.t.}\quad \sum_{i\in\mathcal{S}}\alpha_i y_i=0$$
$$0\leq\alpha_i\leq C,\ \forall i$$

$$\min_{\gamma\geq 0,\ z} C_2\|\gamma\|_p^p+(1-C_2)z$$
$$\text{s.t.}\quad z\geq\min_{\alpha,\nu,\lambda^0,\lambda^C}-\frac{1}{2}\alpha' G_\gamma\alpha+(e-\nu y+\lambda^0-\lambda^C)'\alpha+C(\lambda^C)'e$$
$$\text{s.t.}\quad G_\gamma\alpha-(e-\nu y+\lambda^0-\lambda^C)=0$$
$$\lambda^0,\lambda^C\geq 0$$
$$0\leq\alpha\leq C$$

Recap

$$\min_{\gamma \geq 0} \left[C_2 \|\gamma\|_p^p + (1 - C_2) \max_{\alpha} \sum_{i \in \mathcal{S}} \alpha_i - \frac{1}{2} \sum_{i,\ell \in \mathcal{S}} \alpha_i \alpha_\ell y_i y_\ell K_\gamma(x_i, x_\ell) \right]$$
$$\text{s.t.} \quad \sum_{i \in \mathcal{S}} \alpha_i y_i = 0$$
$$0 \leq \alpha_i \leq C, \forall i$$

$$\min_{\gamma \geq 0, z} C_2 \|\gamma\|_p^p + (1 - C_2) z$$
$$\text{s.t.} \quad z \geq \max_{\alpha} \sum_{i \in \mathcal{S}} \alpha_i - \frac{1}{2} \sum_{i,\ell \in \mathcal{S}} \alpha_i \alpha_\ell y_i y_\ell K_\gamma(x_i, x_\ell)$$
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$$\min_{\gamma \geq 0,\, z} C_2 \|\gamma\|_p^p + (1 - C_2) z$$
$$\text{s.t.} \quad z \geq \min_{\alpha, \nu, \lambda^0, \lambda^C} -\frac{1}{2} \alpha' G_\gamma \alpha + (e - \nu y + \lambda^0 - \lambda^C)' \alpha + C (\lambda^C)' e$$
$$\text{s.t.} \quad G_\gamma \alpha - (e - \nu y + \lambda^0 - \lambda^C) = 0$$
$$\lambda^0, \lambda^C \geq 0$$
$$0 \leq \alpha \leq C$$

$$\min_{\gamma,\, \alpha, \nu, \lambda^0, \lambda^C} C_2 \|\gamma\|_p^p - (1 - C_2) \left(\tfrac{1}{2} \alpha' G_\gamma \alpha - (e - \nu y + \lambda^0 - \lambda^C)' \alpha - C (\lambda^C)' e \right)$$
$$\text{s.t.} \quad G_\gamma \alpha - (e - \nu y + \lambda^0 - \lambda^C) = 0$$
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Outline

How to solve the problem?

- Problem very hard to solve (nonlinear, nonconvex, C, C_2).

$$
\begin{aligned}
\min_{\gamma,\, \alpha, \nu, \lambda^0, \lambda^C} \; & C_2 \|\gamma\|_p^p - (1 - C_2)\left(\tfrac{1}{2}\alpha' G_\gamma \alpha - (e - \nu y + \lambda^0 - \lambda^C)'\alpha - C(\lambda^C)' e\right) \\
\text{s.t. } & G_\gamma \alpha - (e - \nu y + \lambda^0 - \lambda^C) = 0 \\
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\end{aligned}$$

- Simple solving strategy. No ad-hoc approaches.

How to solve the problem?

- Problem very hard to solve (nonlinear, nonconvex, C, C_2).

$$\min_{\gamma,\,\alpha,\nu,\lambda^0,\lambda^C} C_2\|\gamma\|_p^p - (1-C_2)\left(\tfrac{1}{2}\alpha' G_\gamma \alpha - (e - \nu y + \lambda^0 - \lambda^C)'\alpha - C(\lambda^C)'e\right)$$
$$\text{s.t. } G_\gamma \alpha - (e - \nu y + \lambda^0 - \lambda^C) = 0$$
$$\gamma, \lambda^0, \lambda^C \geq 0$$
$$0 \leq \alpha \leq C$$

- Simple solving strategy. No ad-hoc approaches.
- Grid search + local solver (`Ipopt`)+ k-fold CV (train, validation, test).

Experimental Setup

Data set	# individuals	# features	% predominant class
breast	569	30	63%
diabetes	768	8	65%
lymphoma	96	4026	64%
colorectal	62	2000	65%

UCI Machine Learning Repository

Experimental Setup

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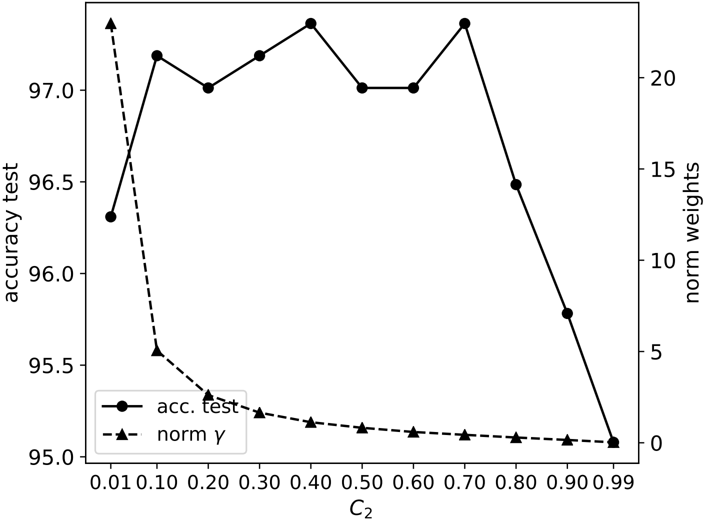
Numerical Results



Numerical Results

	breast
MM-FS	97.35%
NO-FS	97.89%
ℓ_1-SVM	96.83%
Bench. ad-hoc	97.55%
Bench. off-the-shelf	62.74%

Numerical Results

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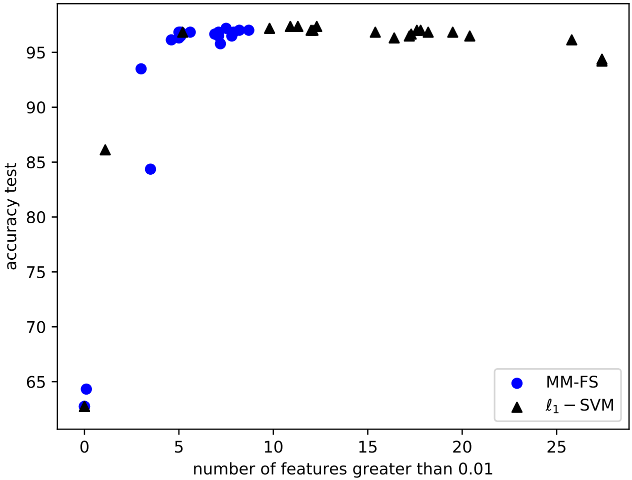

Numerical Results

C_2	0.01	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	0.99
	21	21	21	21	21	21	21	21	21	21	28
	11	22	22	22	22	22	22	22	22	28	21
breast	22	11	8	25	29	28	25	25	28	22	8
	25	7	25	29	25	29	29	29	25	8	23
	30	25	11	8	28	25	28	28	8	7	22

Further info

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Continuous Optimization

A novel embedded min-max approach for feature selection in nonlinear Support Vector Machine classification

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ABSTRACT

In recent years, feature selection has become a challenging problem in several machine learning fields, such as classification problems. Support Vector Machine (SVM) is a well-known technique applied in classification tasks. Various methodologies have been proposed in the literature to select the most relevant features in SVM. Unfortunately, all of them either deal with the feature selection problem in the linear classification setting or propose ad-hoc approaches that are difficult to implement in practice. In contrast, we propose an embedded feature selection method based on a min-max optimization problem, where a trade-off between model complexity and classification accuracy is sought. By leveraging duality theory, we equivalently reformulate the min-max problem and solve it without further ado using off-the-shelf software for nonlinear optimization. The efficiency and usefulness of our approach are tested on several benchmark data sets in terms of accuracy, number of selected features and interpretability.

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Outline

Conclusions

- Min-max optimization problem for SVM classification and feature selection.
- Single-level reformulation based on strong duality.
- Simple but efficient solving strategy. No ad-hoc.
- Competitive literature results.

Conclusions

- Min-max optimization problem for SVM classification and feature selection.
- Single-level reformulation based on strong duality.
- Simple but efficient solving strategy. No ad-hoc.
- Competitive literature results.

Future Research

- Extension to regression or clustering.
- Other real-life applications (Physically-aware approach).

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A novel embedded min-max approach for feature selection in nonlinear Support Vector Machine classification

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Thank you very much for your attention!

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