A min-max approach to feature selection for nonlinear SVM classification.

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Salvador Pineda Morente

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What is OASYS?

OASYS
Optimization and Analytics for Sustainable energY Systems

What is OASYS?

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Combine

- Optimization.
- Data Science.
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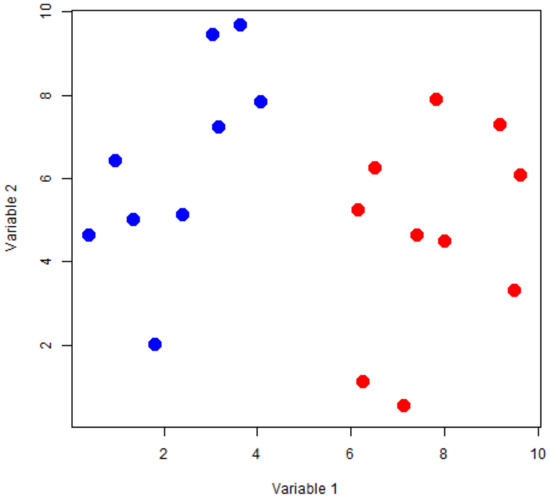
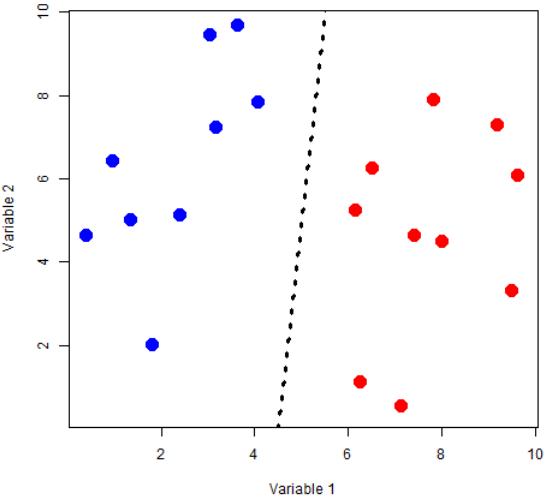
Outline

Outline

Binary Classification Problem.



Binary Classification Problem.



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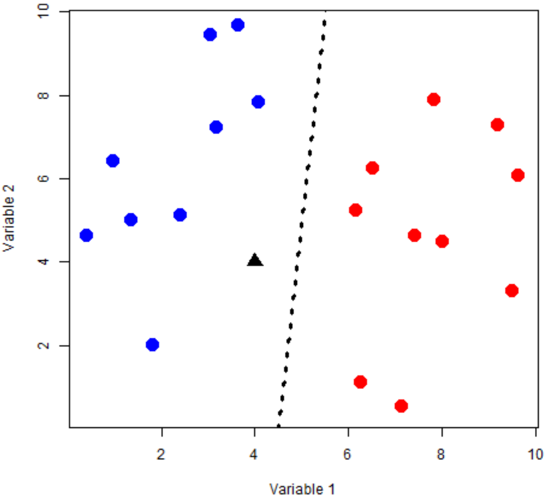

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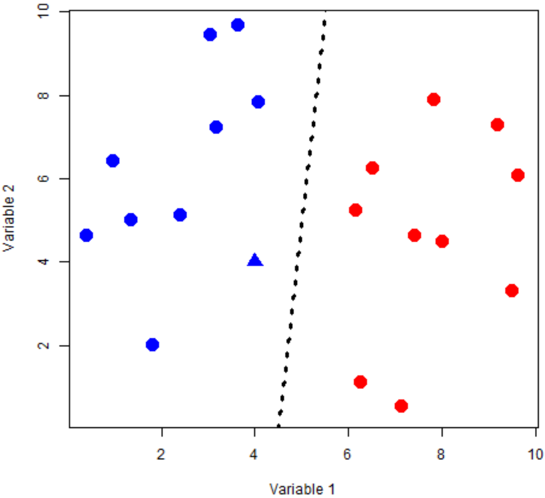
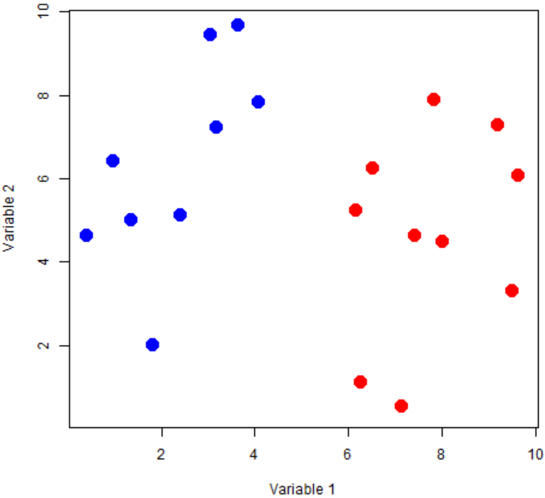


Binary Classification Problem. Feature Selection



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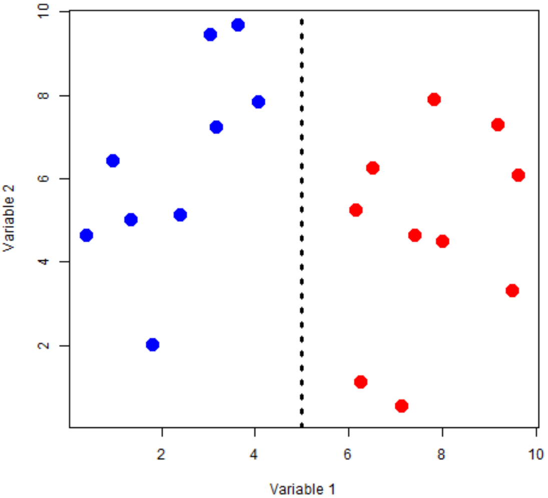

Outline

Aim

- Develop a new mathematical optimization approach to perform feature selection in a binary classification problem.
- Classification tool: nonlinear 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:**
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    - Most separated classes in high-dimensional space.
    - Fast, but not take into account classifier information.

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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.

Literature Review

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    - Wrapper (min-max RFE, *Onel et al. [2019]*):
    - Embedded (KP-SVM, *Maldonado et al. [2011]*):
        - ℓ_0-(pseudo)norm approximation to dual SVM.
        - Large number of hyperparameters.
        - Complicated ad-hoc approaches.

Literature Review

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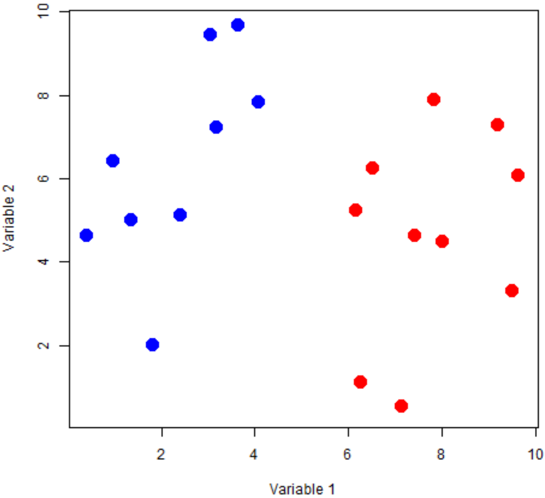
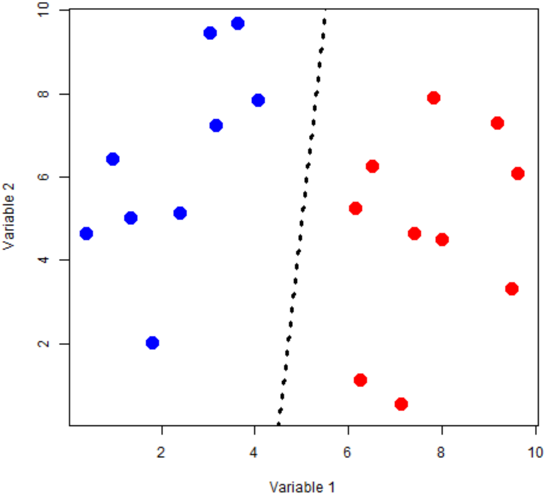
Our contributions

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

SVM



SVM



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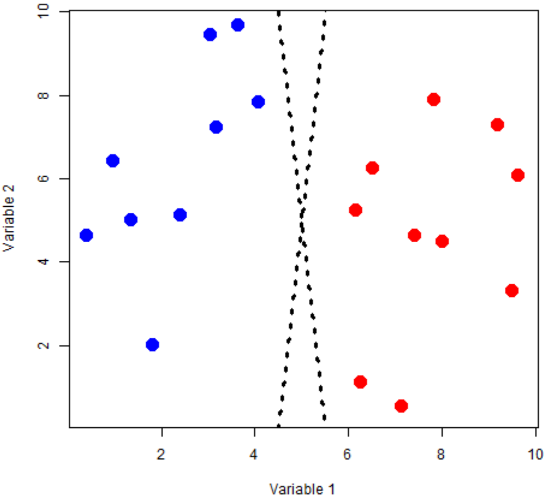

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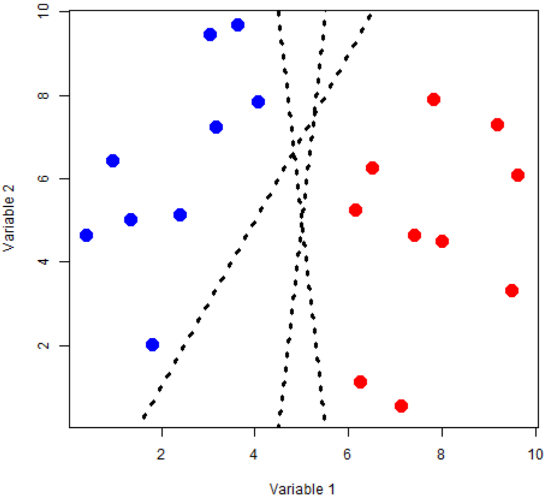
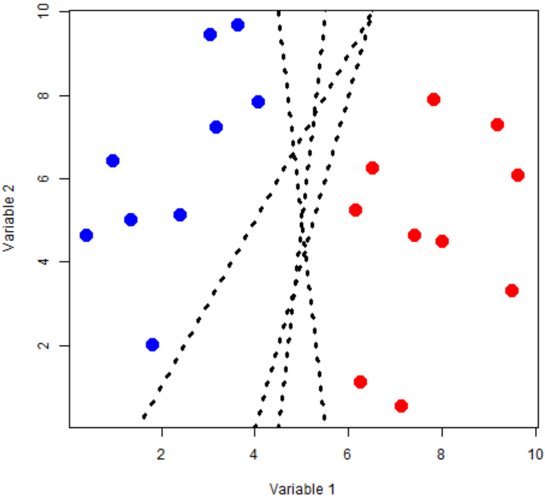
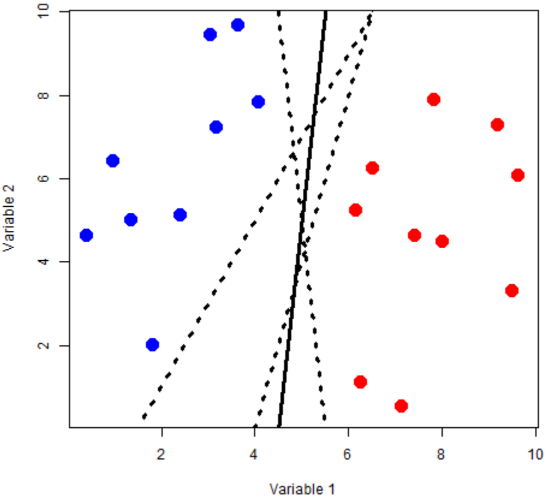


SVM



SVM



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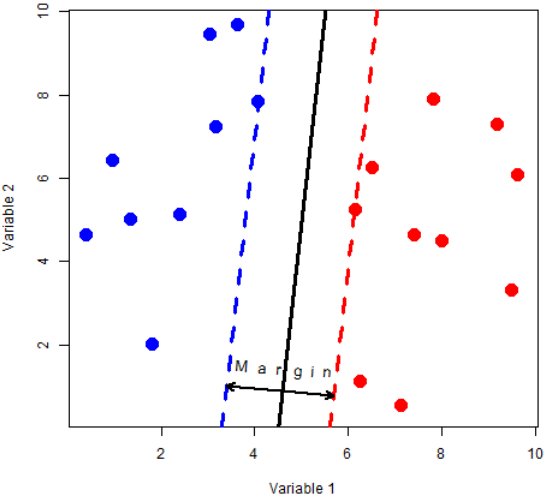

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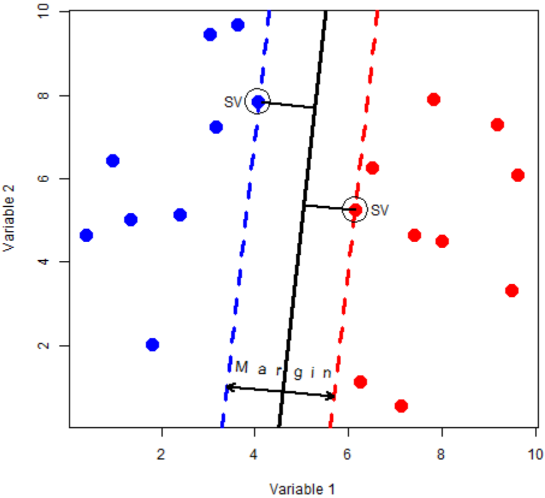

SVM Problem Formulation

Some notation

- Sample $\mathcal{S}$ of individuals.
- Data: $x_i \in \mathbb{R}^M$, $i \in \mathcal{S}$.
- Class label: $y_i \in \{-1, +1\}$, $i \in \mathcal{S}$.
- Hyperplane: $w'x + b = 0$.

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Optimization Problem (Primal)

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

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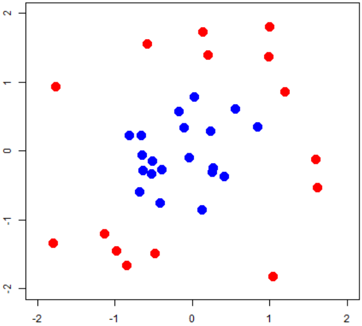
When a new **unseen** individual comes...

Score:

$$\hat{y}(x) = w'x + b$$

x is assigned to class $+1$ iff $\hat{y}(x) > 0$.

What happens in the nonlinear case?



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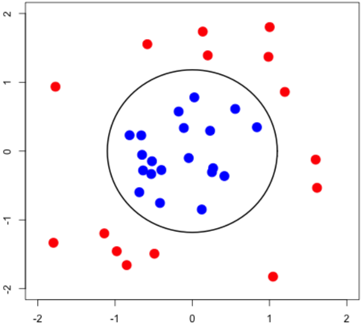

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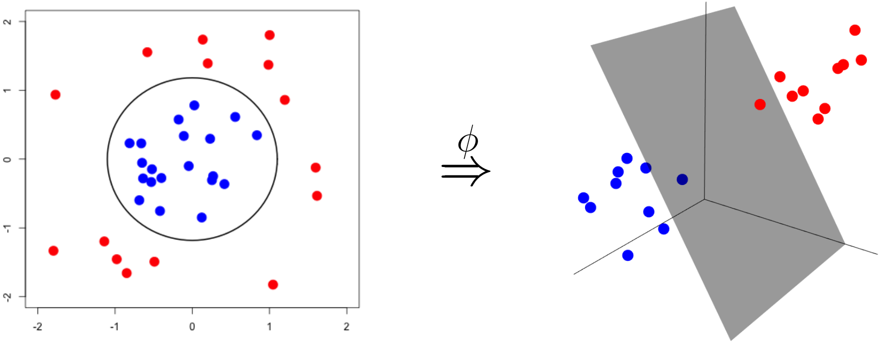

SVM Problem (Primal).

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

SVM Problem (Primal).

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

SVM Problem (Primal). Feature Selection.

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

SVM Problem (Primal). Feature Selection.

$$
\begin{cases}
\min\limits_{\boldsymbol{\gamma}, w, b, \xi} & \frac{1}{2}\|w\|^2 + C\sum\limits_{i \in \mathcal{S}} \xi_i \\
\text{s.t.} & (w' \phi_{\boldsymbol{\gamma}}(x_i) + b) y_i \geq 1 - \xi_i, \quad i \in \mathcal{S} \\
& \xi_i \geq 0, \quad i \in \mathcal{S} \\
& \boldsymbol{\gamma_j \geq 0, \quad \forall j}
\end{cases}
$$

But...

Thanks to the Mercer's theorem, *Mercer [1909]*

SVM Problem (Primal). Feature Selection.

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

Unfortunately

ϕ function is usually unknown.

SVM Problem (Primal). Feature Selection.

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\begin{cases}
\min\limits_{\gamma} \quad \min\limits_{w,b,\xi} & \frac{1}{2}\|w\|^2 + C \sum\limits_{i \in \mathcal{S}} \xi_i \\
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Unfortunately

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SVM Problem (Dual). Feature Selection.

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

SVM Problem (Dual). Feature Selection.

$$\left\{\begin{array}{lll} \min\limits_{\gamma} \max\limits_{\boldsymbol{\alpha}} & \sum\limits_{i \in \mathcal{S}} \boldsymbol{\alpha}_i - \frac{1}{2} \sum\limits_{i,\ell \in \mathcal{S}} \boldsymbol{\alpha}_i \boldsymbol{\alpha}_\ell \boldsymbol{y}_i \boldsymbol{y}_\ell \boldsymbol{\phi}(\boldsymbol{x}_i)' \boldsymbol{\phi}(\boldsymbol{x}_\ell) \\ \text{s.t.} & \sum\limits_{i \in \mathcal{S}} \boldsymbol{\alpha}_i \boldsymbol{y}_i = \mathbf{0} \\ & \boldsymbol{\alpha}_i \in [\mathbf{0}, \boldsymbol{C}], \quad \boldsymbol{i} \in \mathcal{S} \\ & \gamma_j \geq 0, \quad \forall j \end{array}\right.$$

Kernel trick

$$K(x_i, x_\ell) = \phi(x_i)' \phi(x_\ell)$$

SVM Problem (Dual). Feature Selection.

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

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Kernel trick

$$K(x_i, x_\ell) = \phi(x_i)' \phi(x_\ell)$$

Score

$$\hat{y}(x) = \sum_{i \in \mathcal{S}} \alpha_i y_i K(x_i, x)$$

SVM Problem (Dual). Feature Selection.

Anisotropic Gaussian kernel

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

SVM Problem (Dual). Feature Selection.

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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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- $\gamma_j \to \infty$: overfitting.

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Trade-off

- Model complexity.
- Classification accuracy.

Problem Formulation

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

Problem Formulation

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

Problem Formulation

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

Outline

Min-max optimization problem.

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

Epigraph form.

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

Strong duality lower level problem (SVM).

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

Strong duality lower-level problem (SVM).

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

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

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

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

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

Single-level optimization problem

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

Recap

$$\min_{\gamma \geq 0} \left[C_2 \|\gamma\|_p^p + (1 - C_2) \max_{\alpha} \sum_{i \in \mathcal{S}} \alpha_i - \right.$$

$$\left. \frac{1}{2} \sum_{i,\ell \in \mathcal{S}} \alpha_i \alpha_\ell y_i y_\ell K_\gamma(x_i, x_\ell) \right]$$

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

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

Recap

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

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Outline

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

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How to solve the problem?

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$$\text{s.t. } G_\gamma\alpha - (e-\nu y+\lambda^0-\lambda^C) = 0$$
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- Simple solving strategy. No ad-hoc approaches.
- Grid search (C, C_2) + local solver + k-fold CV (train, validation, test).

Outline

Experimental Setup

- UCI Machine Learning Repository, *Dheeru and Karra Taniskidou [2017]*.
- `diabetes` (768 elements, 8 features).
- `breast` (569 elements, 30 features).
- $p = 2$.
- $C \in \{10^{-4}, \ldots, 10^{4}\}$.
- $C_2 \in \{0, 0.1, \ldots, 0.9, 1\}$.
- `Ipopt`.

Numerical Results

diabetes

	Our approach	Literature benchmark (ad-hoc)	Literature benchmark (off-the-shelf)	No feature selection
% accuracy test	77.59 ± 2.29	76.74 ± 1.9	65.11 ± 0.36	77.61 ± 3.32
# selected features ($< 10^{-5}$)	6	5	0	8

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diabetes

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breast

	Our approach	Literature benchmark (ad-hoc)	Literature benchmark (off-the-shelf)	No feature selection
% accuracy test	96.83 ±2.29	97.55±0.9	65.23± 6.19	96.85± 2.41
# selected features ($< 10^{-5}$)	22	15	0	30

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.
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Conclusions

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- Single-level reformulation based on strong duality.
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- Competitive with existing literature results.

Future Research

- Reduce even more the number of features.
- Bigger datasets.
- Extension to regression or clustering.
- Application to Power Systems.

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A min-max approach to feature selection for nonlinear SVM classification.

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Thank you very much for your attention!

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