Support Vector Machine

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Outline

Linear Support Vector Machine

Kernelized SVM

Kernels

From ERM to RLM

Empirical Risk Minimization

in the binary classification case $\mathcal{Y} = \{-1, 1\}$ with the binary loss function

- is computationally hard
- does not provide asymptotic universal consistency

From ERM to RLM

Empirical Risk Minimization

in the binary classification case $\mathcal{Y} = \{-1, 1\}$ with the binary loss function

- is computationally hard
- does not provide asymptotic universal consistency

Regularized Loss Minimization

- replace the binary loss function by a surrogate convex calibrated loss (function)
- add a (convex) regularization term
- typical example: Support Vector Machine

Outline

Linear Support Vector Machine

Kernelized SVM

Kernels

Support Vector Machine (linear case)

Hypotheses

- $\mathcal{Y} = \{-1, 1\}$
- $\mathcal{X} = \mathbb{R}^P$ (with extensions)
- binary loss $l_b(p, t) = \mathbf{1}_{p \neq t}$

RLM point of view

- class of models $\mathcal{G} = \left\{ \mathbf{x} \mapsto g_{\beta_0, \boldsymbol{\beta}}(\mathbf{x}) = \beta_0 + \boldsymbol{\beta}^T \mathbf{x} \right\}$
- surrogate loss: the hinge loss $l_{hinge}(p, t) = \max(0, 1 - pt)$ (convex and calibrated)
- regularization: $\mathbf{C}(g_{\beta_0, \boldsymbol{\beta}}) = \|\boldsymbol{\beta}\|^2$ (convex)

$$\widehat{(\beta_0, \boldsymbol{\beta})} = \arg\min_{\beta_0, \boldsymbol{\beta}} \frac{1}{N} \sum_{i=1}^{N} \max\left(0, 1 - Y_i \left(\beta_0 + \boldsymbol{\beta}^T \mathbf{X}_i\right)\right) + \lambda \|\boldsymbol{\beta}\|^2$$

Ridge principle

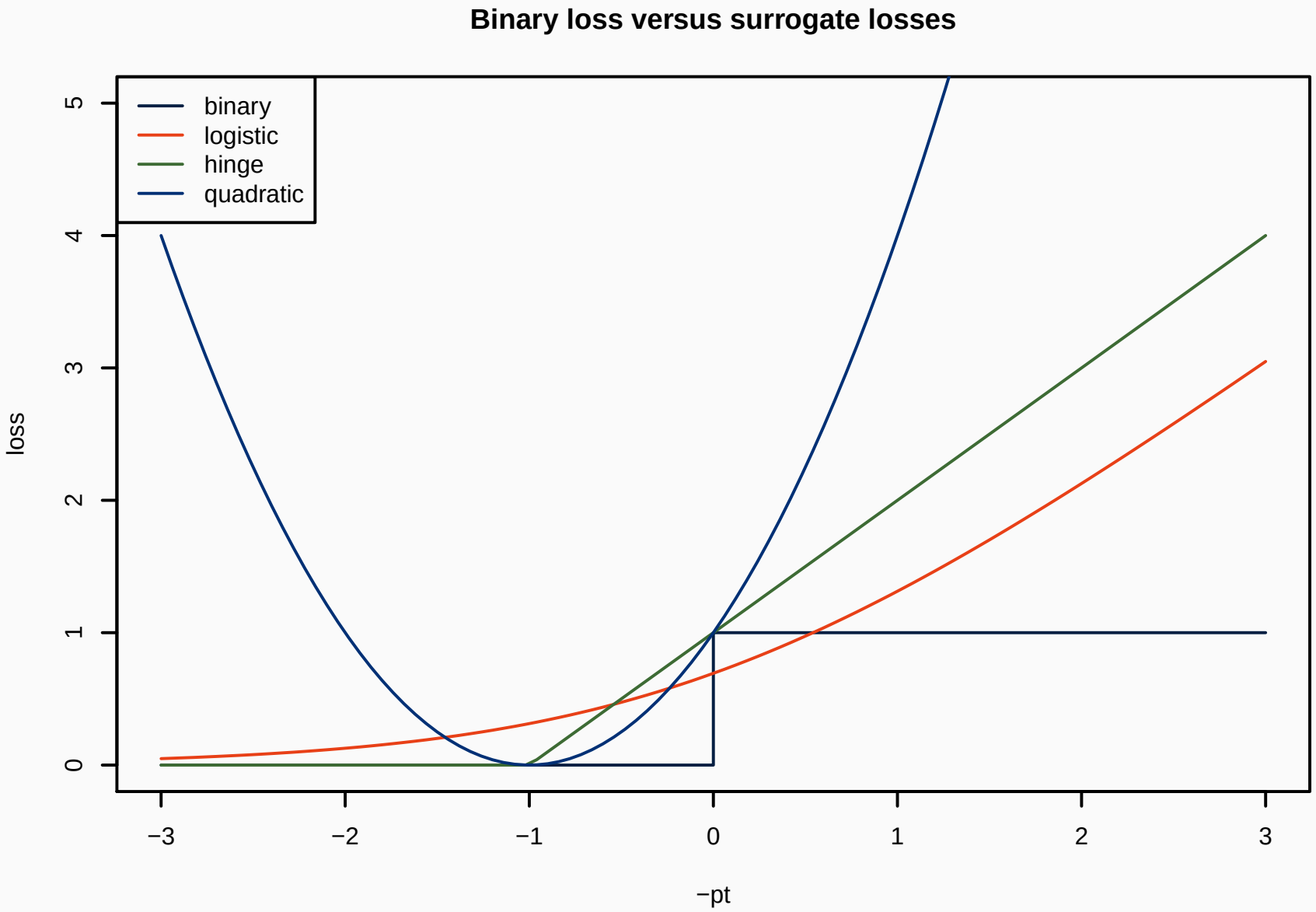
Linear function regularity

- if $f(\mathbf{x}) = \beta^T \mathbf{x}$, then $|f(\mathbf{x}) - f(\mathbf{x}')| \leq \|\beta\| \|\mathbf{x} - \mathbf{x}'\|$ (Cauchy-Schwarz inequality)
- thus $\|\beta\|$ measures the regularity of f

Ridge models

- linear models regularized using their **squared** natural regularity measure
- ridge regression:
  - $\mathcal{Y} = \mathbb{R}$
  - quadratic loss: $l_b(p, t) = (p - t)^2$, no surrogate loss needed
- ridge logistic regression:
  - $\mathcal{Y} = \{-1, 1\}$
  - surrogate logistic loss: $l_{logi}(p, t) = \log(1 + \exp(-pt))$ (convex and calibrated)

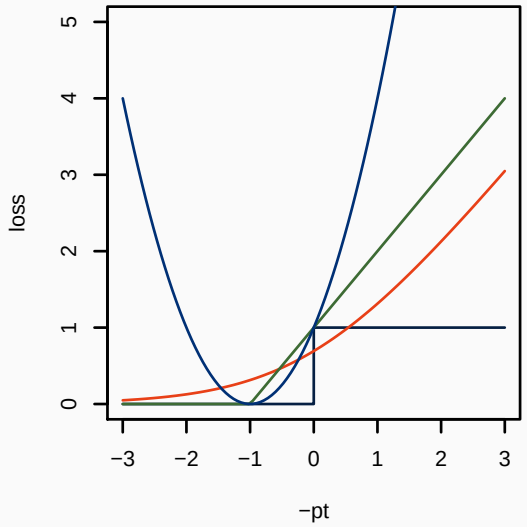
Why the hinge loss?



Why the hinge loss?

The hinge loss

- is convex and calibrated
- is an upper bound of the binary loss
- does not penalize (at all) very good decision ($pt \geq 1$)
- does not overemphasize errors



Robust decisions

- the actual decision model is $f(\mathbf{x}) = \text{sign}(g(\mathbf{x}))$
- if $g(\mathbf{X}_i)\,Y_i \geq 0$ the decision is correct, but it could be influenced by noise, especially is $g(\mathbf{X}_i)\,Y_i \simeq 0$
- confidence in the decision increases with $g(\mathbf{X}_i)\,Y_i$
- the hinge loss penalizes decisions that are not “robust” enough in term of the “margin” $g(\mathbf{X}_i)\,Y_i$

Geometrical point of view

Definition (Linear separation)

A data set $\mathcal{D}$ is **linearly separable** if there is a linear model given by $g_{\beta_0,\boldsymbol{\beta}}(\mathbf{x}) = \beta_0 + \boldsymbol{\beta}^T\mathbf{x}$ such tat $\forall 1 \leq i \leq N$ $\text{sign}(g(\mathbf{X}_i)) = Y_i$

Definition (Geometrical margin)

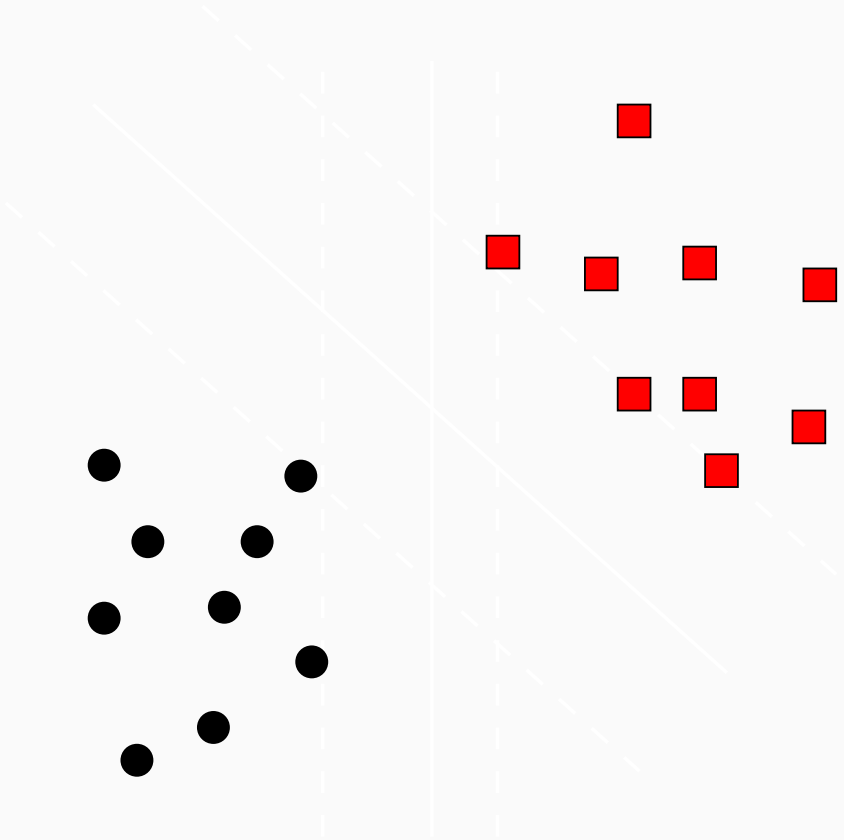
Let $\mathcal{D}$ be a linearly separable data set. The **geometrical margin** of a separating linear model given by $g_{\beta_0,\boldsymbol{\beta}}$ is

$$\mathcal{M}(g_{\beta_0,\boldsymbol{\beta}}) = \min_{1\leq i\leq N} \frac{|\beta_0 + \boldsymbol{\beta}^T\mathbf{X}_i|}{\|\boldsymbol{\beta}\|}.$$

Interpretation

The geometrical margin is the smallest distance between points in the data set and the separating hyperplane associated to the model.

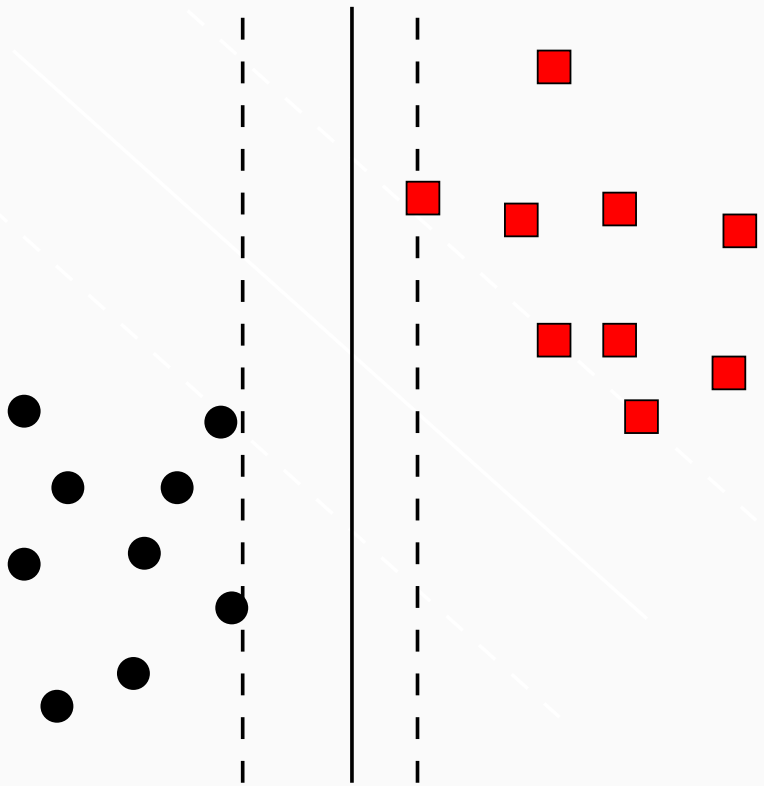
Maximal geometrical margin



Linearly separable data

- many linear classifiers

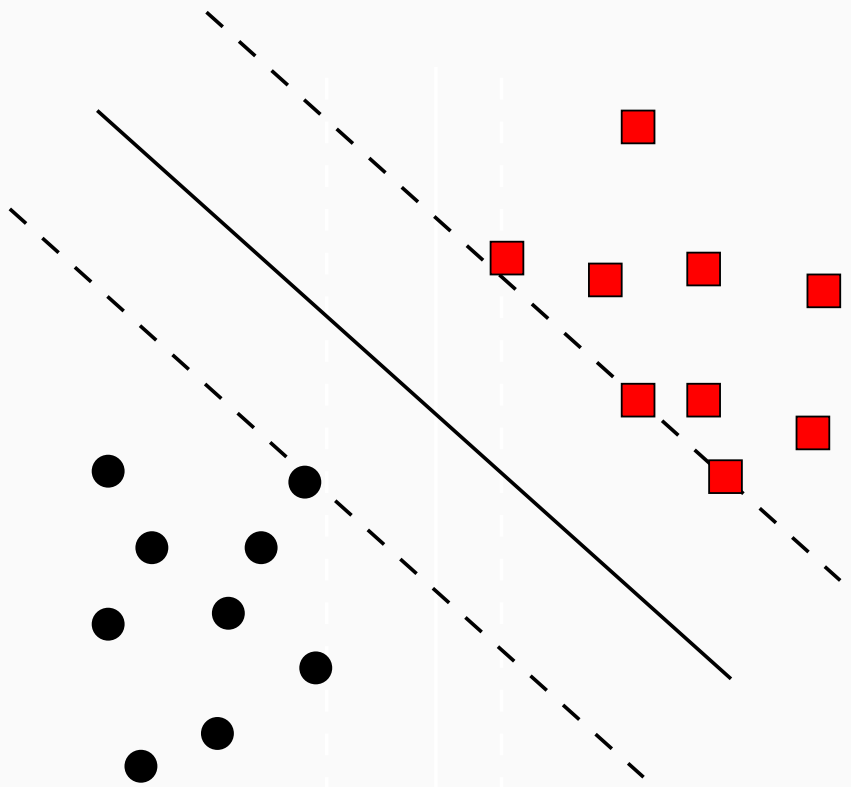
Maximal geometrical margin



Linearly separable data

- many linear classifiers
- if some data are close to the separator, the margin is small $\Rightarrow$ low robustness

Maximal geometrical margin



Linearly separable data

- many linear classifiers
- if some data are close to the separator, the margin is small $\Rightarrow$ low robustness
- choose the classifier by maximizing the geometrical margin

Optimization problem

Geometrical margin maximization

the problem

$$\max_{\beta_0,\boldsymbol{\beta}} \min_{1\leq i\leq N} \frac{|\beta_0 + \boldsymbol{\beta}^T \mathbf{X}_i|}{\|\boldsymbol{\beta}\|}$$

is equivalent to

$$(\mathcal{P}_0) \quad \begin{array}{ll} \underset{\beta_0,\boldsymbol{\beta}}{\text{maximize}} & \min_{1\leq i\leq N} \frac{Y_i(\beta_0+\boldsymbol{\beta}^T \mathbf{X}_i)}{\|\boldsymbol{\beta}\|} \\ \text{subject to} & \forall i,\ Y_i(\beta_0 + \boldsymbol{\beta}^T \mathbf{X}_i) > 0 \end{array}$$

Multiple solutions

- if $(\beta_0, \boldsymbol{\beta})$ is a solution of $(\mathcal{P}_0)$ then $(\lambda\beta_0, \lambda\boldsymbol{\beta})$ is also a solution for any $\lambda > 0$
- normalization needed

Optimization problem

Normalization

- let $(\beta_0, \boldsymbol{\beta})$ be a solution of $(\mathcal{P}_0)$ and denote $\lambda = \min_{1 \leq i \leq N} Y_i(\beta_0 + \boldsymbol{\beta}^T \mathbf{X}_i)$
- as $\lambda > 0$, $(\beta_0', \boldsymbol{\beta}') = \frac{1}{\lambda}(\beta_0, \boldsymbol{\beta})$ is also a solution and

$$\forall i, \ Y_i(\beta_0' + \boldsymbol{\beta}'^T \mathbf{X}_i) = \frac{1}{\lambda} Y_i(\beta_0 + \boldsymbol{\beta}^T \mathbf{X}_i)$$

  and thus $\min_{1 \leq i \leq N} Y_i(\beta_0' + \boldsymbol{\beta}'^T \mathbf{X}_i) = 1$
- the maximal geometrical margin is then $\frac{1}{\|\boldsymbol{\beta}'\|}$
- in summary, if $(\mathcal{P}_0)$ has a solution, then there is $(\beta_0', \boldsymbol{\beta}')$ such that
  - $\min_{1 \leq i \leq N} Y_i(\beta_0' + \boldsymbol{\beta}'^T \mathbf{X}_i) = 1$
  - the margin is $\frac{1}{\|\boldsymbol{\beta}'\|}$

Equivalent problem

Normalized problem

- we consider

$$(\mathcal{P}_1) \quad \underset{\beta_0,\boldsymbol{\beta}}{\text{maximize}} \quad \frac{1}{\|\boldsymbol{\beta}\|} \qquad \text{subject to} \quad \forall i,\ Y_i(\beta_0 + \boldsymbol{\beta}^T \mathbf{X}_i) \geq 1$$

- let $(\beta_0, \boldsymbol{\beta})$ be a solution of $(\mathcal{P}_1)$ and for a $\lambda > 0$ denote $(\beta_0', \boldsymbol{\beta}') = \lambda(\beta_0, \boldsymbol{\beta})$
- then $\frac{1}{\|\boldsymbol{\beta}'\|} = \frac{1}{\lambda\|\boldsymbol{\beta}\|}$ and $\forall i,\ Y_i(\beta_0' + \boldsymbol{\beta}'^T \mathbf{X}_i) \geq \lambda > 0$
- thus $\min_{1\leq i\leq N} \frac{Y_i(\beta_0' + \boldsymbol{\beta}'^T \mathbf{X}_i)}{\|\boldsymbol{\beta}'\|} \geq \frac{1}{\|\boldsymbol{\beta}\|}$
- therefore $(\mathcal{P}_0)$ has a solution with a maximal margin of at least $\frac{1}{\|\boldsymbol{\beta}\|}$
- with the converse result from last slide, we conclude that $(\mathcal{P}_1)$ and $(\mathcal{P}_0)$ have the same optimal value and have solutions together

Linearly separable SVM

Final problem

$$(\mathcal{P}) \quad \underset{\beta_0,\boldsymbol{\beta}}{\text{minimize}} \quad \frac{1}{2}\|\boldsymbol{\beta}\|^2$$
$$\text{subject to} \quad \forall i,\ Y_i(\beta_0 + \boldsymbol{\beta}^T \mathbf{X}_i) \geq 1$$

Convex problem: convex criterion and convex constraints

KKT conditions

- stationarity: $\boldsymbol{\beta}^* = \sum_{i=1}^N \mu_i Y_i \mathbf{X}_i$ and $\sum_{i=1}^N \mu_i Y_i = 0$
- complementary slackness: $\forall i,\ \mu_i \left(Y_i(\beta_0^* + \boldsymbol{\beta}^{*T} \mathbf{X}_i) - 1 \right) = 0$

Support vectors

- the X_i such that $Y_i(\beta_0^* + \boldsymbol{\beta}^{*T} \mathbf{X}_i) = 1$
- $\boldsymbol{\beta}^*$ depends only on them!

Non separable case

Soft margin

- if the data is not separable $\forall i,\ Y_i(\beta_0 + \boldsymbol{\beta}^T \mathbf{X}_i) \geq 1$ can not hold
- relax the constraints: $\forall i,\ Y_i(\beta_0 + \boldsymbol{\beta}^T \mathbf{X}_i) \geq 1 - \xi_i$ (with $\xi_i \geq 0$)
- penalize the relaxation: $\sum_{i=1}^{N} \xi_i$ should be minimal

Linear Support Vector Machine

$$
\begin{array}{lll}
(\mathcal{P}) & \underset{\beta_0, \boldsymbol{\beta}, \boldsymbol{\xi}}{\text{minimize}} & \frac{1}{2}\|\boldsymbol{\beta}\|^2 + C \sum_{i=1}^{N} \xi_i \\
& \text{subject to} & \forall i,\ Y_i(\beta_0 + \boldsymbol{\beta}^T \mathbf{X}_i) \geq 1 - \xi_i \\
& & \forall i,\ \xi_i \geq 0
\end{array}
$$

Link to the hinge loss

Analysis

- let $(\beta_0^*, \boldsymbol{\beta}^*, \boldsymbol{\xi}^*)$ be a solution of $(\mathcal{P})$, then
  - either $\xi_i^* = 0$
  - or $\xi_i^* = 1 - Y_i(\beta_0^* + \boldsymbol{\beta}^{*T}\mathbf{X}_i)$
- and thus $\xi_i^* = \max(0, 1 - Y_i(\beta_0^* + \boldsymbol{\beta}^{*T}\mathbf{X}_i))$
- i.e. $\xi_i^* = l_{hinge}(g_{\beta_0^*, \boldsymbol{\beta}^*}(\mathbf{X}_i), Y_i)$
- therefore solving $(\mathcal{P})$ implies to minimize

$$\frac{1}{2}\|\boldsymbol{\beta}\|^2 + CN\widehat{R}_{l_{hinge}}(g_{\beta_0, \boldsymbol{\beta}}, \mathcal{D})$$

- one can show rigorously that $(\mathcal{P})$ is equivalent to RLM

Dual approach

- $(\mathcal{P})$ is equivalent to following easier to solve dual problem

$$(\mathcal{D}) \quad \underset{\boldsymbol{\alpha}}{\text{maximize}} \quad \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j Y_i Y_j \mathbf{X}_i^T \mathbf{X}_j$$
$$\text{subject to} \quad \sum_{i=1}^{N} \alpha_i Y_i = 0$$
$$\forall i,\ 0 \leq \alpha_i \leq C$$

- for any α_i such that $0 < \alpha_i < C$, $\beta_0 = Y_i - \sum_{j=1}^{N} \alpha_j Y_j \mathbf{X}_i^T \mathbf{X}_j$
- $\boldsymbol{\beta} = \sum_{j=1}^{N} \alpha_j Y_j \mathbf{X}_j$
- conditions on α_i
  - sparsity: $Y_i(\beta_0^* + \boldsymbol{\beta}^{*T} \mathbf{X}_i) > 1 \Rightarrow \alpha_i = 0$
  - support vector: $Y_i(\beta_0^* + \boldsymbol{\beta}^{*T} \mathbf{X}_i) < 1 \Rightarrow \alpha_i = C$
  - on the margin: $0 < \alpha_i < C \Rightarrow Y_i(\beta_0^* + \boldsymbol{\beta}^{*T} \mathbf{X}_i) = 1$

Algorithms

Standard (older) solutions

- with quadratic programming for the dual problem
- scales between $\Theta\left(N^2\right)$ and $\Theta\left(N^3\right)$, depending on the number of support vectors (and thus on C)

Modern approaches

For solutions within ϵ of the optimal one

- cutting plan methods $\Theta\left(\frac{NP}{\lambda\epsilon}\right)$
- stochastic sub-gradient methods $\Theta\left(\frac{P}{\lambda\epsilon}\right)$

Meta-parameter

- C or λ must be optimized (with a validation like approach)
- notice that the running time of the algorithm strongly depends on C/λ

Example

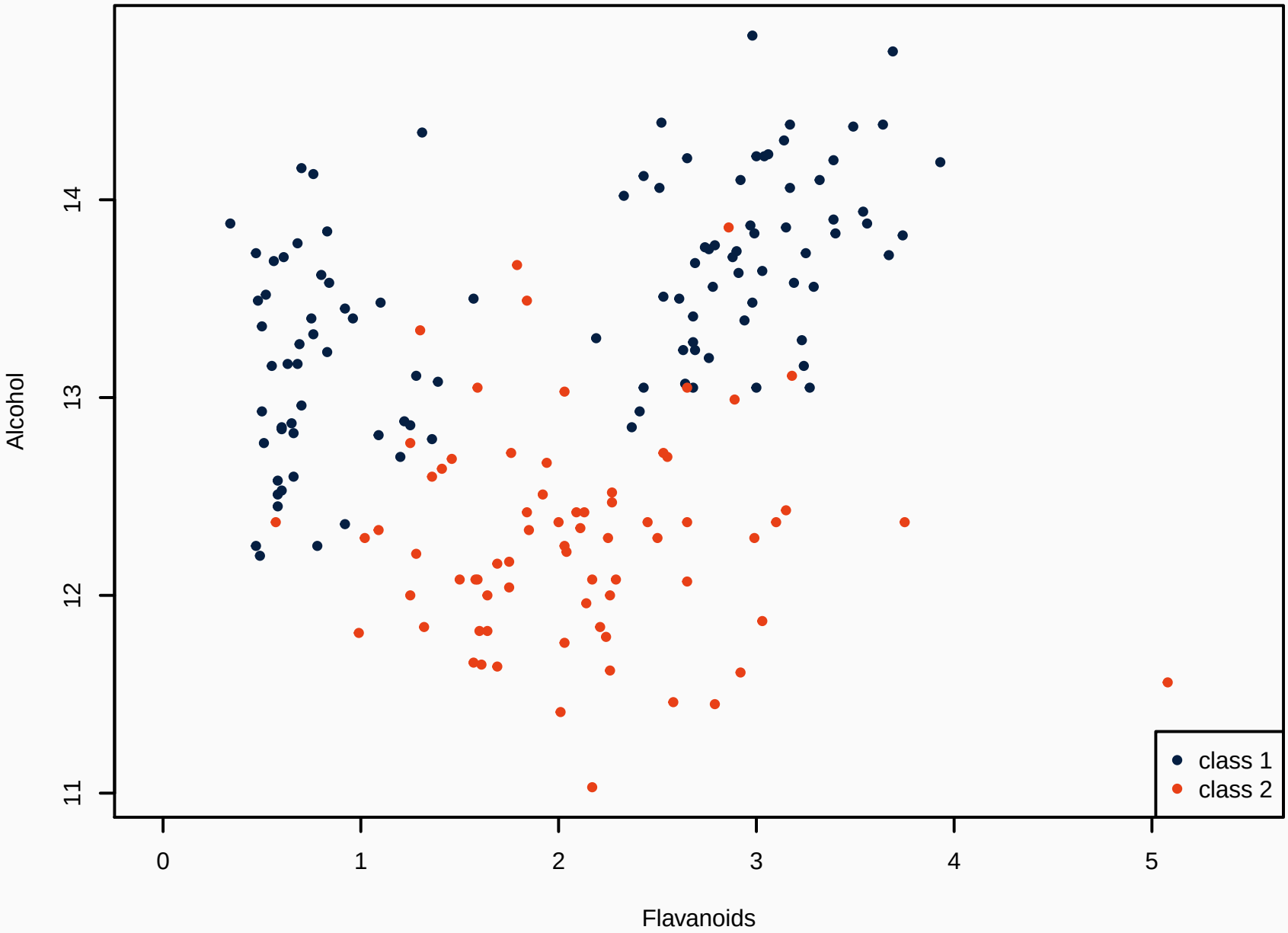
Wine data set

- chemical analysis of wines derived from three cultivars ($\mathcal{Y} = \{1, 2, 3\}$)
- merge cultivar 1 and 3 to get a binary classification problem
- 178 observations with 2 variables ($\mathcal{X} = \mathbb{R}^2$)

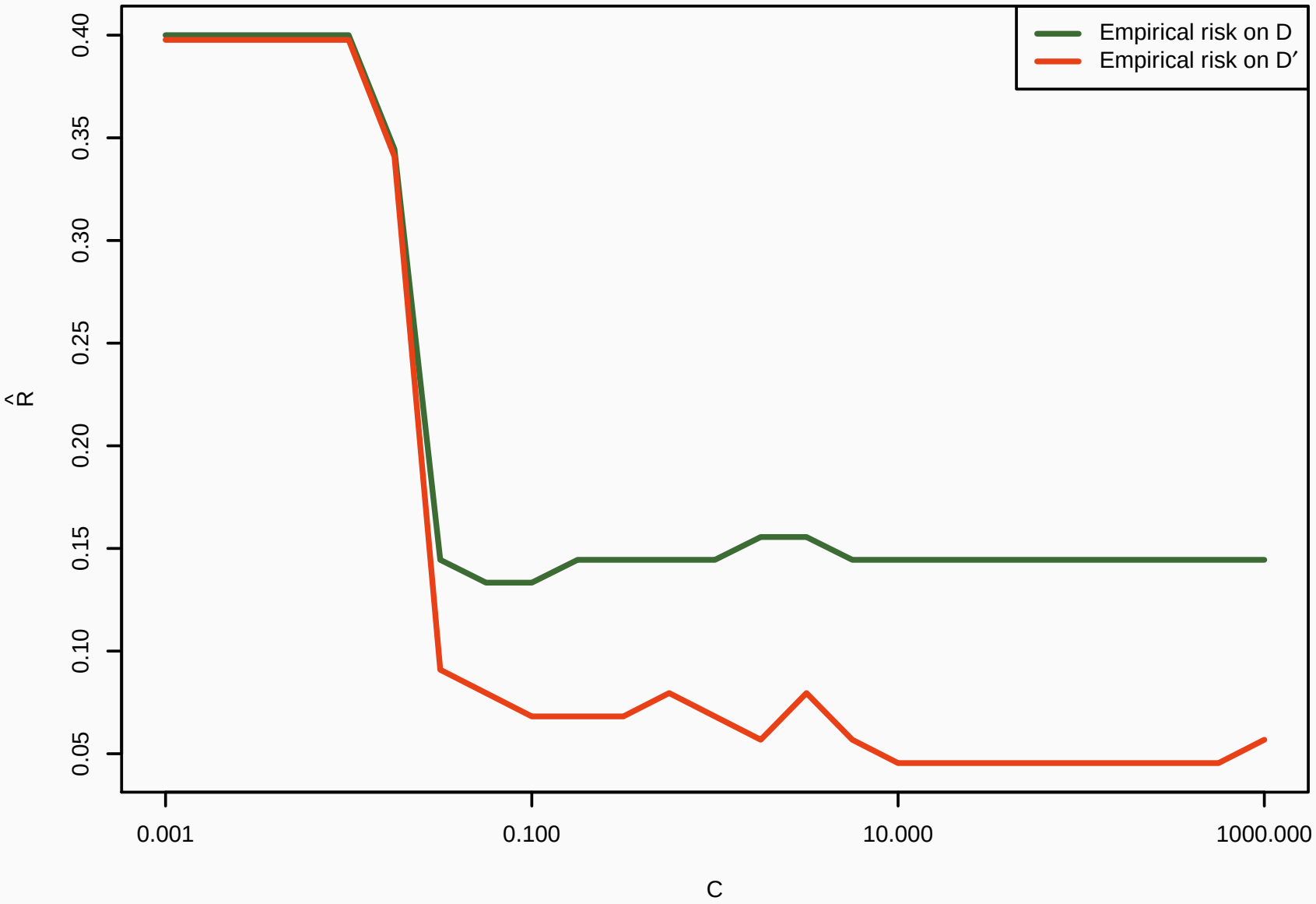
Support vector machine

- use half the data for the learning set $\mathcal{D}$
- use the other half $\mathcal{D}'$ for selecting C
- grid search: C of the form 10^k with $k \in \{-3, -2, \ldots, 3\}$
- notice that the range of C should depend on N

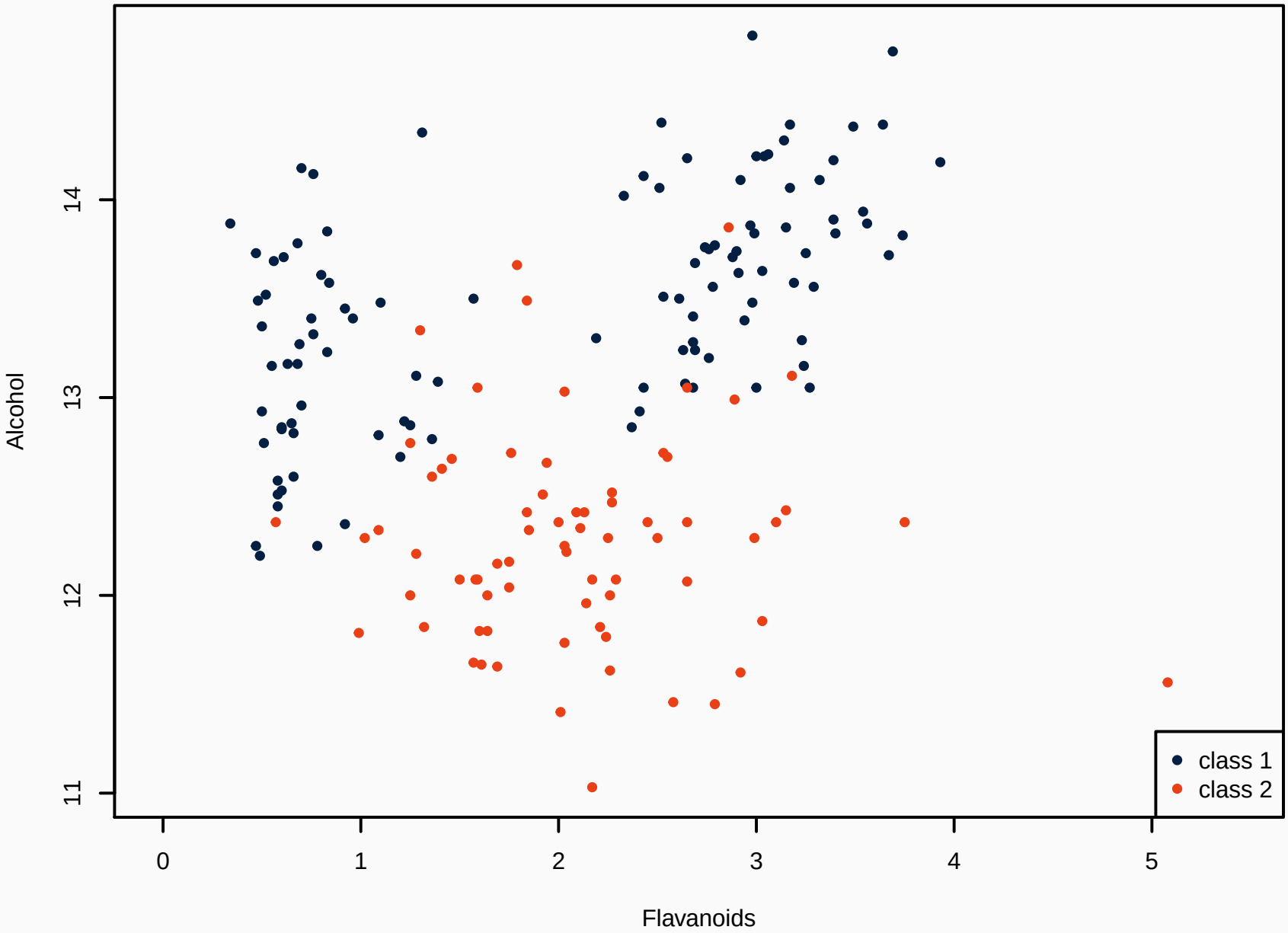
Example



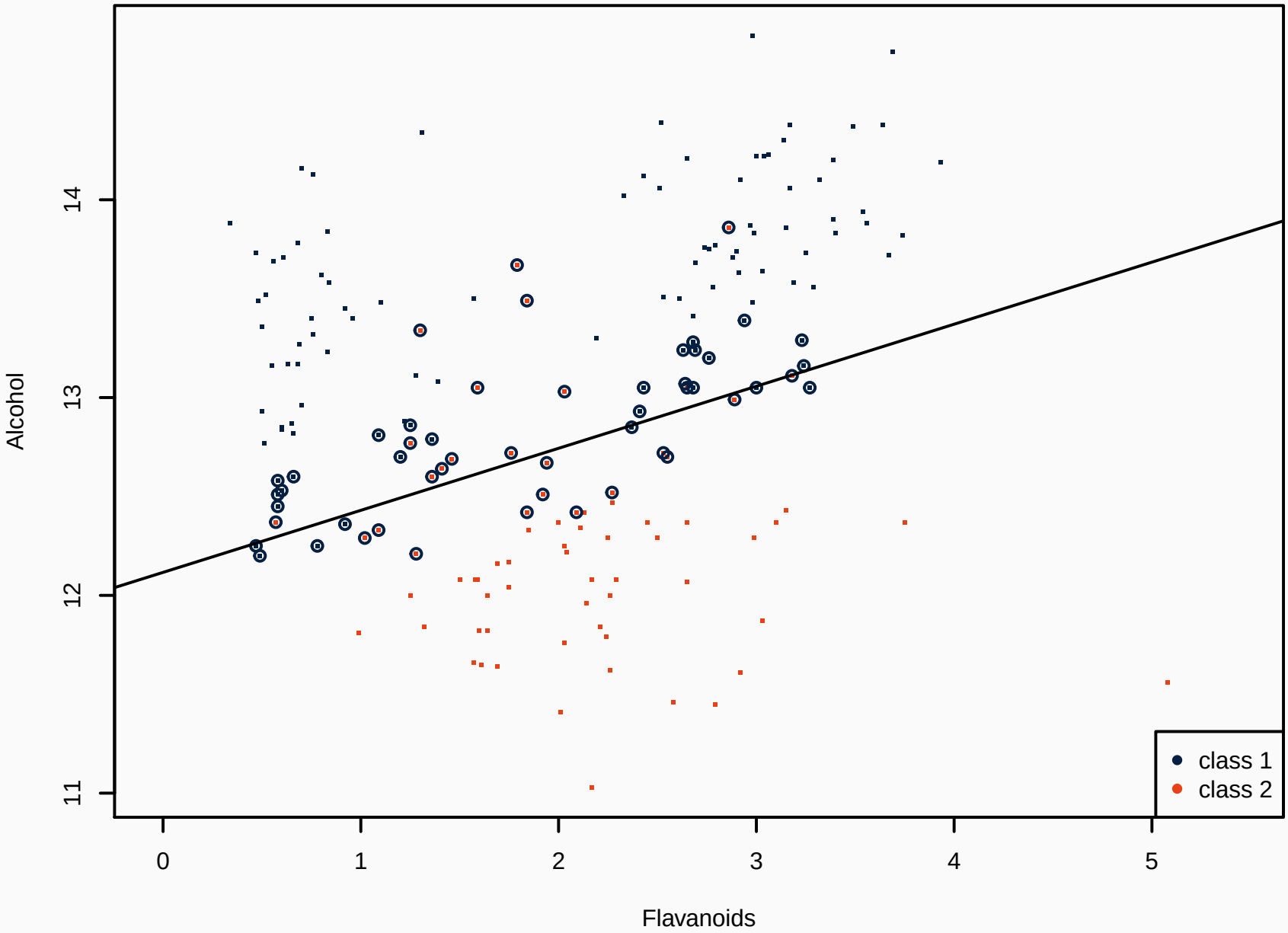
Results


Empirical risk on D
Empirical risk on D′
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
R̂
0.001
0.100
10.000
1000.000
C

Results



Results

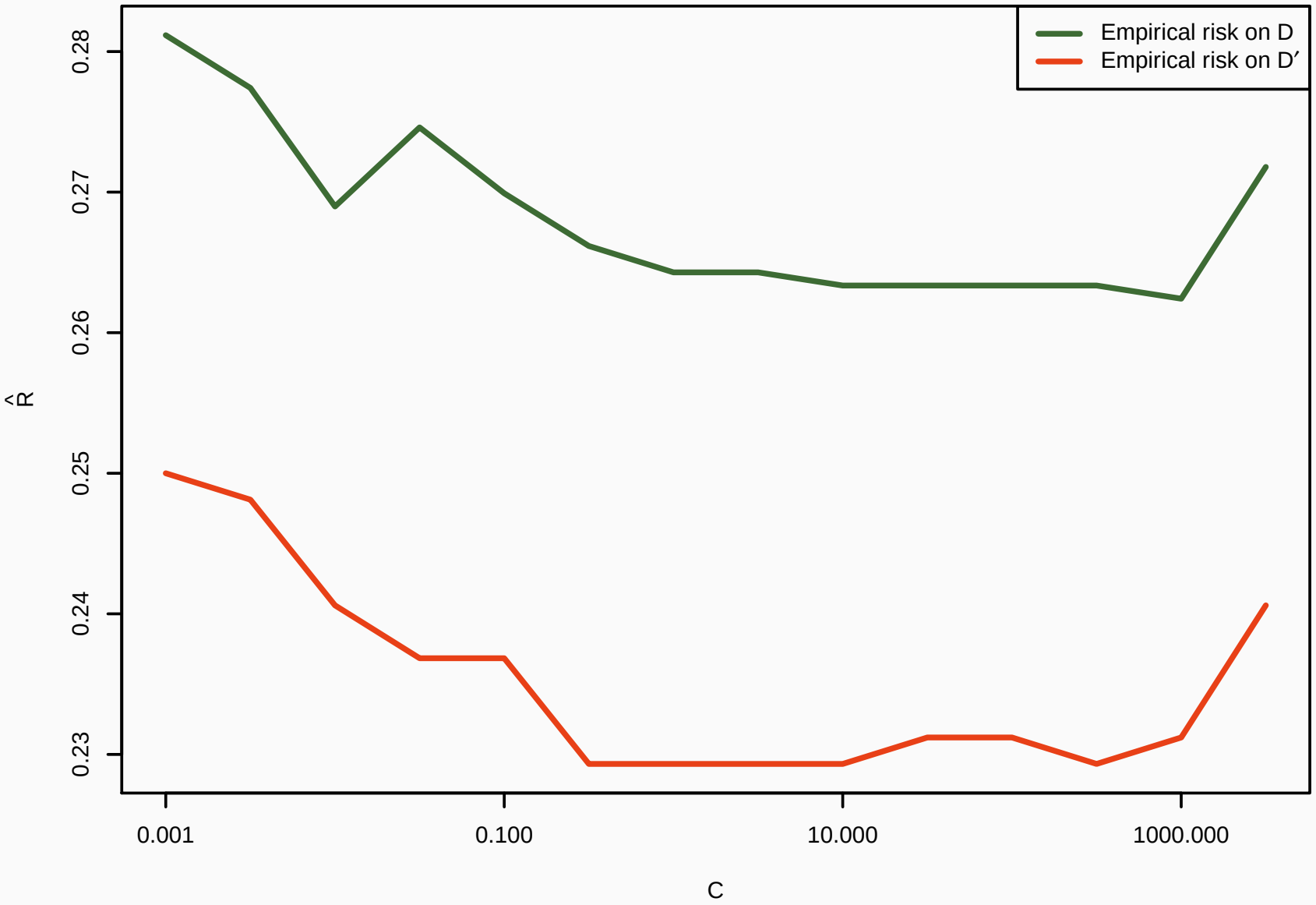


Example

Wine quality data

- quality of a wine graded from 1 to 10:
  - good wines for 6 or more
  - bad wines for 5 or less
- 11 numerical variables giving chemical and physical properties of the wine
- 1067 examples for learning
- 532 examples for selecting C

Results


Empirical risk on D
Empirical risk on D′
0.28
0.27
0.26
0.25
0.24
0.23
R̂
0.001
0.100
10.000
1000.000
C

Results

Confusion matrix

- final model on the full data set

	BAD	GOOD
BAD	574	234
GOOD	170	621

- possible over estimated quality but consistent with the validation set performances

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Linear separability

Are linearly separable data set frequent?

Results from T. Cover (1965) for points in general position:

- separability depends on the dimension of the input space
- the expectation of the maximum number of linearly separable points in dimension P is $2P$
- the expectation of the minimal number of independent variables needed to separate N points is $\frac{N+1}{2}$
- the transition from separable to non separable is more and more abrupt as the dimension increases

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- the expectation of the minimal number of independent variables needed to separate N points is $\frac{N+1}{2}$
- the transition from separable to non separable is more and more abrupt as the dimension increases

Consequence

Let's increase the number of variables!

Explicit mapping

Data transformation

- chose a mapping Φ from $\mathbf{X} = \mathbb{R}^P$ to $\mathbb{R}^Q$ with $Q \gg P$ with $\Phi(\mathbf{X}) = (\phi_1(\mathbf{X}), \ldots, \phi_Q(\mathbf{X}))^T$
- replace the data set $\mathcal{D} = ((\mathbf{X}_i, \mathbf{Y}_i))_{1 \leq i \leq N}$ by $((\Phi(\mathbf{X}_i), \mathbf{Y}_i))_{1 \leq i \leq N}$
- classical approach for the generalized linear model with
  - interaction terms $\phi(\mathbf{X}) = X_j \times X_k$
  - polynomial terms $\phi(\mathbf{X}) = X_j^k$
  - etc.

Support Vector Machine

- applies directly with $g_{\beta_0, \boldsymbol{\beta}}(\mathbf{x}) = \beta_0 + \boldsymbol{\beta}^T \Phi(\mathbf{x})$
- can be used with $Q = N$ by leveraging the regularization (as in ridge regression)

SVM optimization revisited

Primal version

$$(\mathcal{P}) \quad \underset{\beta_0,\boldsymbol{\beta},\boldsymbol{\xi}}{\text{minimize}} \quad \frac{1}{2}\|\boldsymbol{\beta}\|^2 + C\sum_{i=1}^{N}\xi_i$$
$$\text{subject to} \quad \forall i,\ Y_i(\beta_0 + \boldsymbol{\beta}^T\Phi(\mathbf{X}_i)) \geq 1 - \xi_i$$
$$\forall i,\ \xi_i \geq 0$$

The parameter number grows with Q

Dual version

$$(\mathcal{D}) \quad \underset{\boldsymbol{\alpha}}{\text{maximize}} \quad \sum_{i=1}^{N}\alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\alpha_i\alpha_j Y_i Y_j \Phi(\mathbf{X}_i)^T\Phi(\mathbf{X}_j)$$
$$\text{subject to} \quad \sum_{i=1}^{N}\alpha_i Y_i = 0$$
$$\forall i,\ 0 \leq \alpha_i \leq C$$

The α parameter dimension does not depend on Q

SVM optimization revisited

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The α parameter dimension does not depend on Q

Dual problem

Representation of the solution

- $\beta_0 = Y_i - \sum_{j=1}^{N} \alpha_j \Phi(\mathbf{X}_i)^T \Phi(\mathbf{X}_j)$ for an α_i such that $0 < \alpha_i < C$
- $\boldsymbol{\beta} = \sum_{j=1}^{N} \alpha_j Y_j \Phi(\mathbf{X}_j)$ and therefore

$$g_{\beta_0,\boldsymbol{\beta}}(\mathbf{x}) = \beta_0 + \sum_{j=1}^{N} \alpha_j Y_j \Phi(\mathbf{X}_j)^T \Phi(\mathbf{x}) = g_{\beta_0,\boldsymbol{\alpha}}(\mathbf{x})$$

Calculating the SVM

- $\boldsymbol{\beta}$ is not needed
- the parameters β_0 and $\boldsymbol{\alpha}$ are of fixed dimension independent of Q
- everything can be computed using only $\Phi(\mathbf{x})^T \Phi(\mathbf{x}')$ for $\mathbf{x} \in \mathcal{X}$ and $\mathbf{x}' \in \mathcal{X}$

Dual problem

Representation of the solution

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Regularization point of view

Regularization term

- original term $\|\beta\|^2$
- using the formula for β we have

$$\|\beta\|^2 = \sum_{i=1}^{N}\sum_{j=1}^{N} \alpha_i \alpha_j Y_i Y_j \Phi(\mathbf{X}_i)^T \Phi(\mathbf{X}_j)$$

Hinge loss

$$\widehat{R}_{l_{hinge}}(g_{\beta_0,\boldsymbol{\alpha}}, \mathcal{D}) = \frac{1}{N}\sum_{i=1}^{N} \max\left(0, 1 - Y_i\left(\beta_0 + \sum_{j=1}^{N} \alpha_j Y_j \Phi(\mathbf{X}_j)^T \Phi(\mathbf{X}_i)\right)\right)$$

Regularization point of view

Regularization term

- original term $\|\beta\|^2$
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$$\|\beta\|^2 = \sum_{i=1}^{N}\sum_{j=1}^{N} \alpha_i \alpha_j Y_i Y_j \Phi(\mathbf{X}_i)^T \Phi(\mathbf{X}_j)$$

Hinge loss

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Implicit approach

Specifying Φ

- with the dual problem or the regularization approach we do not need Φ but rather $\Phi(\mathbf{x})^T\Phi(\mathbf{x}')$ for any $(\mathbf{x}, \mathbf{x}') \in \mathcal{X}^2$
- the linear case corresponds to $\Phi(\mathbf{x})^T\Phi(\mathbf{x}') = \mathbf{x}^T\mathbf{x}'$
- could we specify directly $k(\mathbf{x}, \mathbf{x}')$?

Definition (Kernel)

A kernel K on a set $\mathcal{X}$ is a function from $\mathcal{X} \times \mathcal{X}$ to $\mathbb{R}$ such that

- k is **symmetric**: $\forall(\mathbf{x}, \mathbf{x}') \in \mathcal{X} \times \mathcal{X}$, $k(\mathbf{x}, \mathbf{x}') = k(\mathbf{x}', \mathbf{x})$
- k is **positive definite**: for all $n \geq 1$, all $(\mathbf{x}_i)_{1 \leq i \leq n}$, n elements of $\mathcal{X}$, and all $(\gamma_i)_{1 \leq i \leq n}$, n elements of $\mathbb{R}$,

$$\sum_{i=1}^{n}\sum_{j=1}^{n} \gamma_i\gamma_j k(\mathbf{x}_i, \mathbf{x}_j) \geq 0$$

Kernel based SVM

Dual with kernel

- optimization problem

$$(\mathcal{D}) \quad \underset{\boldsymbol{\alpha}}{\text{maximize}} \quad \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j Y_i Y_j k(\mathbf{X}_i, \mathbf{X}_j)$$
$$\text{subject to} \quad \sum_{i=1}^{N} \alpha_i Y_i = 0$$
$$\forall i,\ 0 \leq \alpha_i \leq C$$

- $\beta_0 = Y_i - \sum_{j=1}^{N} \alpha_j k(\mathbf{X}_i, \mathbf{X}_j)$
- model

$$g_{\beta_0, \boldsymbol{\alpha}}(\mathbf{x}) = \beta_0 + \sum_{j=1}^{N} \alpha_j Y_j k(\mathbf{X}_j, \mathbf{x})$$

- similar construction for the regularized point of view

Issues

Important questions

- Does this construction make sense?
- Why specifying a kernel k rather than a transformation Φ?

Outline

Linear Support Vector Machine

Kernelized SVM

Kernels

Kernels are efficient

Polynomial kernel

- for $\mathcal{X} = \mathbb{R}^P$, $k_d(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^T\mathbf{x}' + 1)^d$ is a kernel
- computation time $\Theta(P + d)$
- one can show that there is Φ_d from $\mathcal{X}$ to $\mathbb{R}^Q$ such that $k_d(\mathbf{x}, \mathbf{x}') = \Phi_d(\mathbf{x})^T\Phi_d(\mathbf{x}')$
- but $Q = \binom{P+d}{P} = \frac{(P+d)!}{P!d!}$ and computing Φ costs a lot, e.g. $\Theta\left(P^d\right)$ when d is small and P is large

Illustration

- for $d = 2$ and $P = 2$, $\Phi_2(\mathbf{x}) = \left(1, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1x_2, x_1^2, x_2^2\right)^T$
- $\Phi_2(\mathbf{x})$ computation involves 6 operations and $\Phi_2(\mathbf{x})^T\Phi_2(\mathbf{x}')$ uses 11 operations
- $k_2(\mathbf{x}, \mathbf{x}')$ needs 5 operations

Kernels are flexible

Numerical examples

For $\mathcal{X} = \mathbb{R}^P$

- Linear kernel: $k_{lin}(\mathbf{x}, \mathbf{x}') = \mathbf{x}^T\mathbf{x}'$
- Polynomial kernel: $k_d(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^T\mathbf{x}' + 1)^d$
- Gaussian kernel: $k_{gauss,\sigma}(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x}-\mathbf{x}'\|^2}{2\sigma^2}\right)$
- Laplace kernel: $k_{lap,\gamma}(\mathbf{x}, \mathbf{x}') = \exp\left(-\gamma\|\mathbf{x} - \mathbf{x}'\|\right)$

Dissimilarity spaces

When $\mathcal{X}$ has a dissimilarity d, one can use the Gaussian kernel as follows: $k_{gauss,\sigma}(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{d(\mathbf{x},\mathbf{x}')}{2\sigma^2}\right)$

Kernels are flexible

String kernels

For $\mathcal{X}$ the set of words on an alphabet Σ (i.e., $\mathcal{X} = \Sigma^*$)

- generic matching kernel
  $k(\mathbf{x}, \mathbf{x}') = \sum_{s \in \sigma^*} \text{num}(\mathbf{x}, s)\text{num}(\mathbf{x}', s)w(s)$ where $\text{num}(\mathbf{x}, s)$ denotes the number of times a string s occurs in $\mathbf{x}$ and $w(s)$ is a weighting function on Σ^*
- examples:
  - common characters: $w(s) = 0$ is $|s| > 1$ (where $|s|$ is the length of the string s)
  - common sub-strings or words with similar tricks
- numerous extensions: position dependent weighting, approximate matches, etc.

Kernels are flexible

Many other input types

- graph nodes
- whole graphs
- texts
- images
- etc.

Kernel theory

Definition (Reproducing Kernel Hilbert Space (RKHS))

Let $\mathcal{X}$ be an arbitrary space and let H be a Hilbert space of functions from $\mathcal{X}$ to $\mathbb{R}$ (with the inner product $\langle ., . \rangle_H$). H is a Reproducing Kernel Hilbert Space if there is a function K from $\mathcal{X} \times \mathcal{X}$ to $\mathbb{R}$ such that:

1. for all $\mathbf{x} \in \mathcal{X}$, $K(\mathbf{x}, .) \in H$
2. for all $f \in H$ and for all $\mathbf{x} \in \mathcal{X}$, $f(x) = \langle f, K(\mathbf{x}, .) \rangle_H$

K is the reproducing kernel of H.

Theorem (Moore–Aronszajn)

Let k be a symmetric positive definite kernel on $\mathcal{X}$. Then there is a unique RKHS of functions from $\mathcal{X}$ to $\mathbb{R}$ for which k is the reproducing kernel.

From theory to practice

Kernel trick

Assume given a symmetric positive definite kernel k on $\mathcal{X}$.

- then there is a **feature space** H and a **feature map** Φ from $\mathcal{X}$ to H defined by $\Phi(\mathbf{x}) = k(\mathbf{x}, .)$
- H is a vector space with an inner product: any machine learning algorithm that uses only the Euclidean structure of $\mathbb{R}^P$ can be implemented in H
- for instance the linear SVM:
  - replace $\beta^T \mathbf{x}$ by $\langle \beta, \Phi(\mathbf{x}) \rangle_H$
  - and $\|\beta\|^2$ by $\|\beta\|_H^2$

Representer theorem

To ease the use of the kernel trick, we need a theorem.

Theorem (Representer theorem)

Let k be a symmetric positive definite kernel on $\mathcal{X}$ with H the associated RKHS. Assume that C is a strictly increasing function from $\mathbb{R}^+$ to $\mathbb{R}$ and R is a function from $\mathbb{R}^N$ to $\mathbb{R}$. Any solution to

$$\arg\min_{f \in H} R(f(\mathbf{x}_1), \ldots, f(\mathbf{x}_N)) + C(\|f\|_H)$$

for some fixed elements of $\mathcal{X}$, $\mathbf{x}_1, \ldots, \mathbf{x}_N$, can be written $f = \sum_{i=1}^{N} \alpha_i k(\mathbf{x}_i, .)$

Livear SVM and the kernel trick

Regularized version

- optimization problem with $\boldsymbol{\beta} \in H$

$$\min_{\beta_0, \boldsymbol{\beta}} \frac{1}{N} \sum_{i=1}^{N} l_{hinge} \left(\beta_0 + \langle \boldsymbol{\beta}, \Phi(\mathbf{X}_i) \rangle_H, Y_i\right) + \lambda \|\boldsymbol{\beta}\|_H^2$$

  with $\Phi(\mathbf{X}_i) = k(\mathbf{X}_i, .)$
- according to the representer theorem, $\boldsymbol{\beta}$ has the form $\sum_{j=1}^{N} \alpha_j k(\mathbf{X}_j, .)$ and therefore
  - $\langle \boldsymbol{\beta}, \Phi(\mathbf{X}_i) \rangle_H = \sum_{j=1}^{N} \alpha_j \langle k(\mathbf{X}_j, .), k(\mathbf{X}_i, .) \rangle_H = \sum_{j=1}^{N} \alpha_j k(\mathbf{X}_i, \mathbf{X}_j)$
  - $\|\boldsymbol{\beta}\|_H^2 = \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j k(\mathbf{X}_i, \mathbf{X}_j)$
- new optimization problem

$$\min_{\beta_0, \boldsymbol{\alpha}} \frac{1}{N} \sum_{i=1}^{N} l_{hinge} \left(\beta_0 + \sum_{j=1}^{N} \alpha_j k(\mathbf{X}_i, \mathbf{X}_j), Y_i \right) + \lambda \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j k(\mathbf{X}_i, \mathbf{X}_j)$$

Kernel ridge regression

Ridge regression

- regularized linear regression
- optimization problem in an arbitrary Hilbert space H

$$\min_{\beta_0,\boldsymbol{\beta}} \frac{1}{N}\sum_{i=1}^{N}(\beta_0 + \langle\boldsymbol{\beta}, \Phi(\mathbf{X}_i)\rangle_H - Y_i)^2 + \lambda\|\boldsymbol{\beta}\|_H$$

Kernel ridge regression

- representer theorem again!
- transformed optimization problem

$$\min_{\beta_0,\boldsymbol{\alpha}} \frac{1}{N}\sum_{i=1}^{N}\left(\beta_0 + \sum_{j=1}^{N}\alpha_j k(\mathbf{X}_i, \mathbf{X}_j) - Y_i\right)^2 + \lambda\sum_{i=1}^{N}\sum_{j=1}^{N}\alpha_i\alpha_j k(\mathbf{X}_i, \mathbf{X}_j)$$

Kernels provide consistent learning

Dimension

- many kernels increase a lot the dimension of the data representation
- some kernels lead to a RHKS of infinite dimension (e.g., the Gaussian kernel)
- according to Cover's theorem, this should turn any data set into a linearly separable one
- but interesting RHKS have infinite VC-dimension!

Effect of regularization

- in the convex case $g^* = \arg\min_{\{g \in H | \|g\|_H \leq \mu\}} \widehat{A}(g, \mathcal{D})$
- even if H has an infinite VC-dimension, $\{g \in H | \|g\|_H \leq \mu\}$ has a controlled capacity
- consistency can be proved in some cases (e.g. SVM)

General framework

- chose a kernel k
- chose a loss function l
- chose a penalty function $\mathbf{C}$ (strictly increasing function)
- solve

$$\min_{\beta_0,\boldsymbol{\alpha}} \frac{1}{N}\sum_{i=1}^{N} l\left(\beta_0 + \sum_{j=1}^{N}\alpha_j k(\mathbf{X}_i,\mathbf{X}_j), Y_i\right) + \lambda \mathbf{C}\left(\sum_{i=1}^{N}\sum_{j=1}^{N}\alpha_i\alpha_j k(\mathbf{X}_i,\mathbf{X}_j)\right)$$

- use a model derived from (or equal to) $\mathbf{X} \mapsto \beta_0 + \sum_{j=1}^{N}\alpha_j k(\mathbf{X}_i,\mathbf{X})$
- very general consistent results are available
- very good performances in practice

In practice

Practical aspects

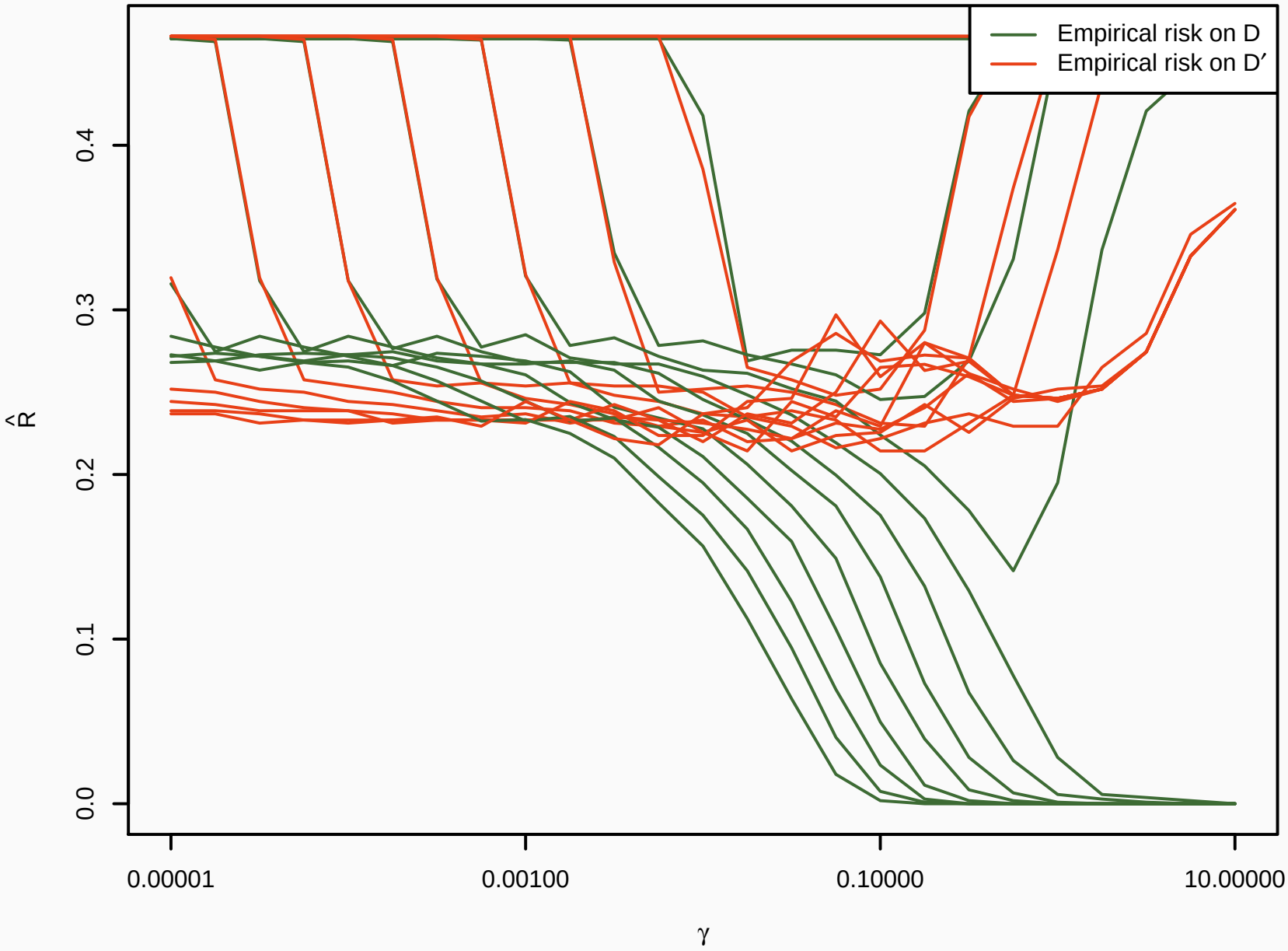
- loss functions?
  - quadratic in regression
  - hinge loss in classification
  - numerous other possibilities
- kernel?
  - must be chosen by a validation like approach
  - meta parameter(s) must be tuned
  - the Gaussian kernel is the de facto standard choice
- the regularization trade-off must be tuned by a validation like approach

Example

Wine quality data

- Same setting as before
  - quality of a wine graded from 1 to 10:
    - good wines for 6 or more
    - bad wines for 5 or less
  - 11 numerical variables giving chemical and physical properties of the wine
  - 1067 examples for learning
  - 532 examples for selecting C
- SVM with the hinge loss and a Gaussian kernel
- in R with e1071, the Gaussian kernel is $k(\mathbf{x}, \mathbf{x}') = \exp(-\gamma \|\mathbf{x} - \mathbf{x}'\|^2)$

Results


Empirical risk on D
Empirical risk on D′
0.0
0.1
0.2
0.3
0.4
R̂
0.00001
0.00100
0.10000
10.00000
γ

Results

Confusion matrix

- final model on the full data set

	BAD	GOOD
BAD	574	234
GOOD	170	621

Linear kernel

	BAD	GOOD
BAD	584	184
GOOD	160	671

Gaussian kernel

- possible over estimated quality but consistent with the validation set performances

Remarks

- strong overfitting when C is large and γ also
- somewhat similar effects of C and γ: small values favor regular models, large values favor overfitting

Outline

Linear Support Vector Machine

Kernelized SVM

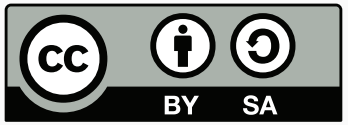
Kernels

Summary

Kernel methods

- a general framework for convex regularized loss minimization
- pros and cons
  - \+ very flexible framework (regression, classification, but also semi-supervised learning, novelty detection, etc)
  - \+ can be applied to exotic data with adapted kernels
  - \+ state of the art performances
  - \+ strong theoretical results
  - \- relatively slow especially for nonlinear kernels
  - \- many meta-parameters
  - \- somewhat complex implementations

Licence



Version

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