Support Vector Machines

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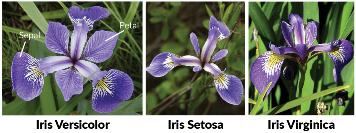
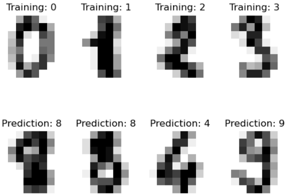
Classification I

Principle

Identify the category of an object

- Binary classification: Positive or Negative, $0, 1$ or $-1, 1$ (Breast Cancer,Spam detection, ...)
- Multi classification: More than 2 classes (object classification, iris: plant species, ...)





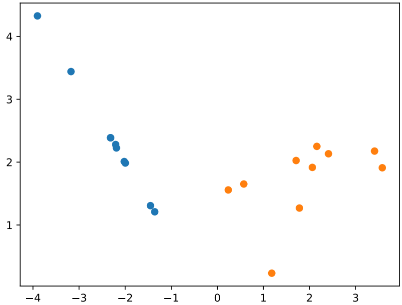
Classification II

Formally

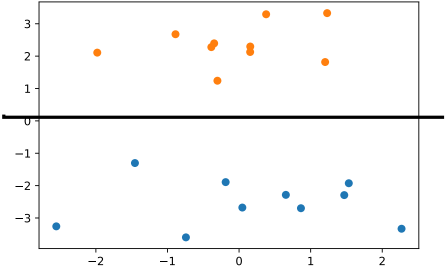
- Dataset $\mathcal{D} = \{(\mathbf{x}_i, y_i) \in \mathcal{X} \times \mathcal{Y}\}_{i=1...N}$ with $\mathcal{Y} \in \{-1, 1\}$
- Prediction function f:
  - $f : \mathcal{X} \to \{-1, 1\}$
  - $f : \mathcal{X} \to \mathbb{R} : \begin{cases} f(\mathbf{x}) > 0 \to 1 \\ f(\mathbf{x}) < 0 \to -1 \end{cases}$
- Metrics: Accuracy, precision, recall, AUC, ...

Linearly separable problem

It exists at least one line which separates the data in two classes (in 2D)



Linear Classifier



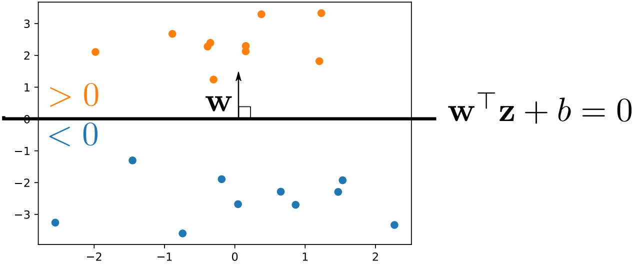
- Find a separator between classes
- Parameters of model : $\boldsymbol{w} \in \mathbb{R}^d, b \in \mathbb{R}$
- Decision function:

$$f(\mathbf{x}) = \boldsymbol{w}^\top \mathbf{x} + b \begin{cases} f(\mathbf{x}) > 0 \rightarrow 1 \\ f(\mathbf{x}) < 0 \rightarrow -1 \end{cases}$$

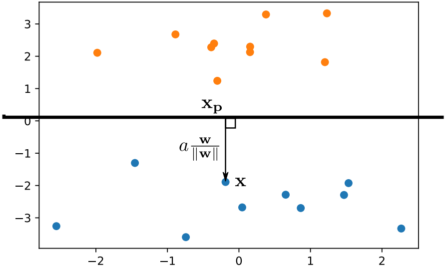
Hyperplane

Hyperplane $\mathcal{H}_{\boldsymbol{w},b}$:

$$\mathcal{H}_{\boldsymbol{w},b} = \{\boldsymbol{z} \in R^d | f(\boldsymbol{z}) = \boldsymbol{w}^\top \boldsymbol{z} + b = 0\}$$



Distance to the hyperplane



$$\begin{aligned} \mathbf{x} &= \mathbf{x}_p + a\frac{\boldsymbol{w}}{\|\boldsymbol{w}\|} \\ \Rightarrow \quad a &= \frac{\boldsymbol{w}^\top \mathbf{x} + b}{\|\boldsymbol{w}\|} \end{aligned}$$

Proof

Distance $d(\mathcal{H}, \mathbf{x})$

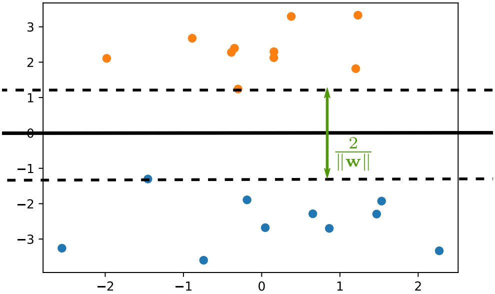
$$d(\mathcal{H}, \mathbf{x}) = |a| = \frac{|\boldsymbol{w}^\top \mathbf{x} + b|}{\|\boldsymbol{w}\|}$$

Definition of margin

Margin

- Minimum distance between a point and $\mathcal{H}$
- Canonical hyperplane :

$$\min_{\mathbf{x}_i \forall i \in 1 \dots N} \boldsymbol{w}^\top \mathbf{x}_i + b = 1$$



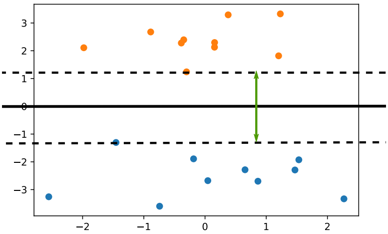
Maximization of margin

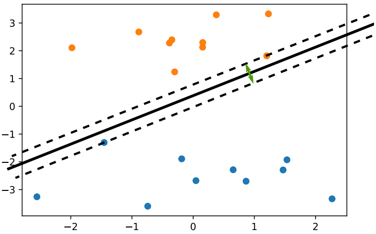
Better classifier separates the data

- Many different hyperplanes separate the data
- How to select the best ?
- $\Rightarrow$ Maximize the margin

Maximization of the margin

- Maximize the margin $\Leftrightarrow$ maximize $\frac{2}{\|\boldsymbol{w}\|}$
- $\boldsymbol{w}^\star = \operatorname{argmin}_{\boldsymbol{w}} \|\boldsymbol{w}\|$





Linear Separable SVM

Principle of SVM

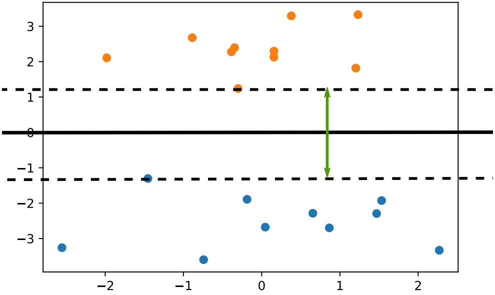
Find an hyperplane $\mathcal{H}$ which :

- separates well the data

$$y_i f(\mathbf{x}_i) > 1, \forall i \in 1 \dots N$$

- maximizes the margin

$$\underset{\boldsymbol{w}}{\operatorname{argmin}} \|\boldsymbol{w}\|^2$$



Objective function

Hard-margin

$$\min_{\boldsymbol{w},b} \quad \frac{1}{2}\|\boldsymbol{w}\|^2$$

s.t.

$$y_i(\boldsymbol{w}^\top \mathbf{x}_i + b) \geq 1, \forall i \in 1 \dots N$$

Control + data term

Data term

$$y_i(\boldsymbol{w}^\top \mathbf{x}_i + b) \geq 1$$

- N Constraints
- Ensures that the train set is separated

Control term

$$\|\boldsymbol{w}\|^2$$

- Maximize the margin
- Selects the "best" model

How to resolve the SVM problem ?

Constraints

- We know how to optimize $\|\boldsymbol{w}\|^2$
- But the constraints ?

Solution

- Transform the problem
- Use Lagrangian dual

Lagrangian equivalence

Lagrangian

- Dual formulation of a constrained optimization problem
- Transform constraints to term
- Introduction of Lagrange multipliers for each constraint

Lagrangian of SVM

$$\mathcal{L}(\boldsymbol{w}, b, \alpha) = \frac{1}{2}\|\boldsymbol{w}\|^2 - \sum_{i=1}^{N} \alpha_i (y_i(\boldsymbol{w}^\top \mathbf{x}_i + b) - 1)$$

Dual problem I

Dual SVM problem

- Annilihate the gradient wrt to primal variables
- Rewrite $\mathcal{L}(\boldsymbol{w}, b, \alpha)$ to eliminate primal variables
- Minimizing primal $\Leftrightarrow$ maximizing dual

$$\max_{\alpha} \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^\top \mathbf{x}_j$$

s. t.

$$\alpha_i \geq 0, \forall i \in 1 \dots N$$

$$\sum_{i=1}^{N} \alpha_i y_i = 0$$

Dual problem II

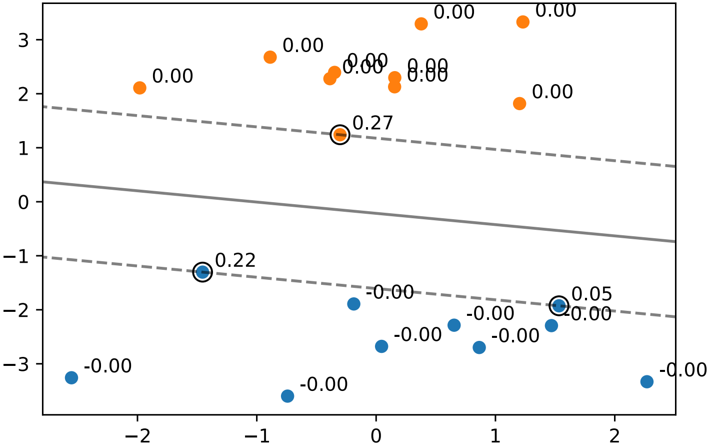
Resolving dual formulation

- Quadratic programming (use a solver)
- Compute optimal $\alpha^\star$

Dual variables α

- $\alpha^\star \in \mathbb{R}^N$ is the solution of dual SVM
- $\alpha_i^\star \neq 0$ for x_i in the margin
- $\alpha_i^\star = 0$ else.

Support vectors



Classification function

Retrieving $\boldsymbol{w}$

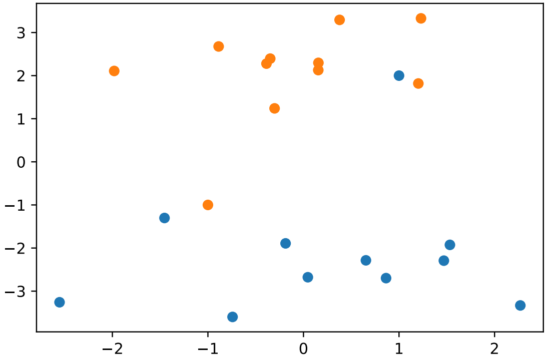
- $\boldsymbol{w} = \sum_{i=1}^{N} \alpha_i \boldsymbol{y}_i \mathbf{x}_i$
- Decision function $f(\mathbf{x}')$

$$f(\mathbf{x}') = \boldsymbol{w}^\top \mathbf{x}' + b = \sum_{i=1}^{N} \alpha_i \boldsymbol{y}_i \mathbf{x}_i^\top \mathbf{x}' + b$$

Observations

- No need of $\boldsymbol{w}$ to predict
- Only scalar product between data
- Only few support vectors (sparsity)

How to deal with non separable case ?



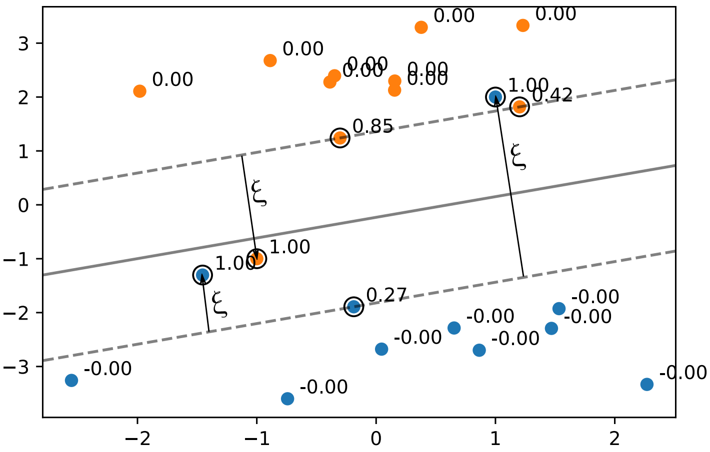
The ξ slack variables

Allow some errors

- Relax the margin by allowing errors
- Constraints:
$$\boldsymbol{y}_i(\boldsymbol{w}^\top \mathbf{x}_i + b) \geq 1 - \xi_i$$
- $\xi_i \geq 0$

Must be minimized

- Fit to data term
- We want to minimize the errors
- $\min \sum_i \xi_i$



0.00
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1.00
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1.00
ξ
0.27
-0.00
-0.00
-0.00
-0.00
-0.00
-0.00
-0.00
-0.00
3
2
1
0
−1
−2
−3
−2
−1
0
1
2

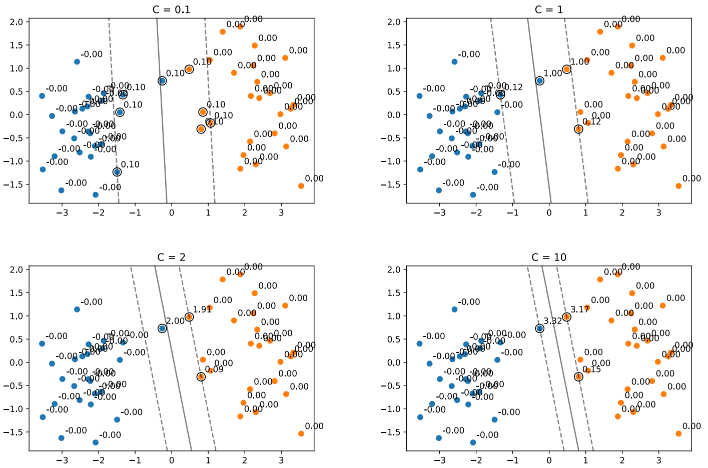
SVM-C Objective function

$$\min_{\boldsymbol{w},b} \quad \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{i=1}^{N}\xi_i$$

s.t.

$$\begin{aligned} & y_i(\boldsymbol{w}^\top \mathbf{x}_i + b) \geq 1 - \xi_i && ,\forall i \in 1 \ldots N \\ & \xi_i \geq 0 && ,\forall i \in 1 \ldots N \end{aligned}$$

- $C > 0$
- C balances the regularization and fit to data term
- Big C : small errors, small margin
- Low C : big errors, big margin



C = 0.1
C = 1
C = 2
C = 10

Dual formulation

Support vector values

- $0 \leq \alpha_i \leq C$

C parameter

- Controls the balance regularization/fit to data term
- Needs to be tuned

Let's try it

SVM for Regression : SVR

Regression

Regression problem

- Dataset $\mathcal{D} = \{(\mathbf{x}_i, y_i) \in \mathcal{X} \times \mathcal{Y}\}_{i=1\ldots N}$ with $\mathcal{Y} \in \mathbb{R}$
- Prediction function f:

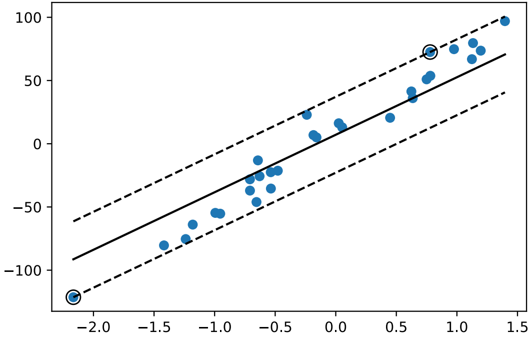
$$f(\mathbf{x}_i) = \boldsymbol{w}^\top \mathbf{x}_i + b \simeq \boldsymbol{y}_i$$

- Metrics: RMSE, MAE, R^2, ...
- Methods: Kernel Ridge Regression, ...

From classification to regression

How to adapt margin to regression ?

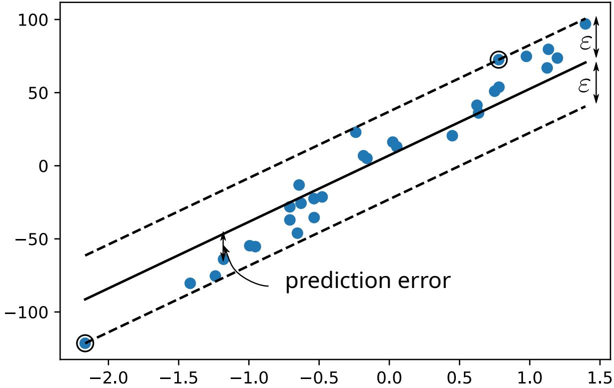
- We must gather the data
- We don't want to split
- How to ?



Adapting margin to regression

Solution

- Margin: contains the data
- $\boldsymbol{w}^\top \mathbf{x}_i + b \simeq y_i \Leftrightarrow \boldsymbol{w}^\top \mathbf{x}_i + b = y_i \pm \varepsilon$
- Adapt the size of margin ε to contain the data



SVR Objective function

SVR problem formulation

$$
\begin{aligned}
\min_{\boldsymbol{w},b} \quad & \frac{1}{2}\|\boldsymbol{w}\|^2 \\
\text{s t.} \quad & y_i - \boldsymbol{w}^\top x_i - b \le \varepsilon, \forall i \in 1 \dots N \\
& \boldsymbol{w}^\top x_i + b - y_i \le \varepsilon, \forall i \in 1 \dots N
\end{aligned}
$$

- $2N$ constraints
- ε insensitive cost

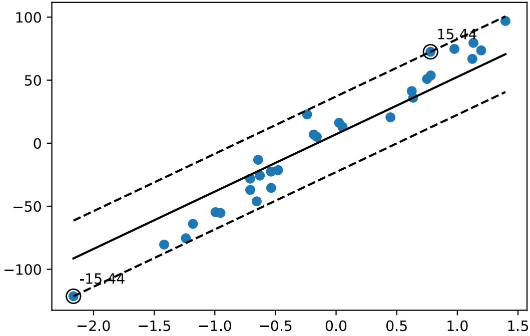
Hyperparameters

- ε : define the size of the margin
- Condition: it exists $\boldsymbol{w}, b$ which contains the data within ε.

Resolution

Dual variables

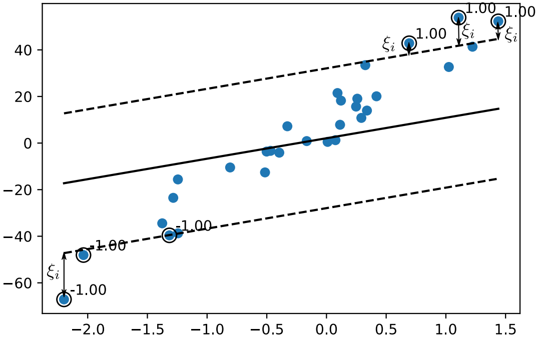
- $2N$ dual variables : $\alpha_i, \alpha^\star \geq 0$,
- One vector can be only on one margin
- $\alpha_i \neq 0 \Rightarrow \alpha_i^\star = 0$, and vice versa
- Constraint satisfied : $\alpha_i^{(\star)} = 0$



SVR with errors

Integrating errors

- Allowing to be outside the margin
- Manage outliers
- Relax the constraints with ξ_i values



SVR objective function I

Primal

$$
\begin{aligned}
\min_{\boldsymbol{w},b} \quad & \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{i=1}^{N}(\xi_i + \xi_i^\star) & \\
\text{s. t.} \quad & y_i - \boldsymbol{w}^\top x_i - b \leq \varepsilon + \xi_i & , \forall i \in 1 \dots N \\
& \boldsymbol{w}^\top x_i + b - y_i \leq \varepsilon + \xi_i^\star & , \forall i \in 1 \dots N \\
& \xi_i, \xi_i^\star \geq 0 & , \forall i \in 1 \dots N
\end{aligned}
$$

- $4N$ constraints
- New hyperparameter: $C \geq 0$

Dual Resolution

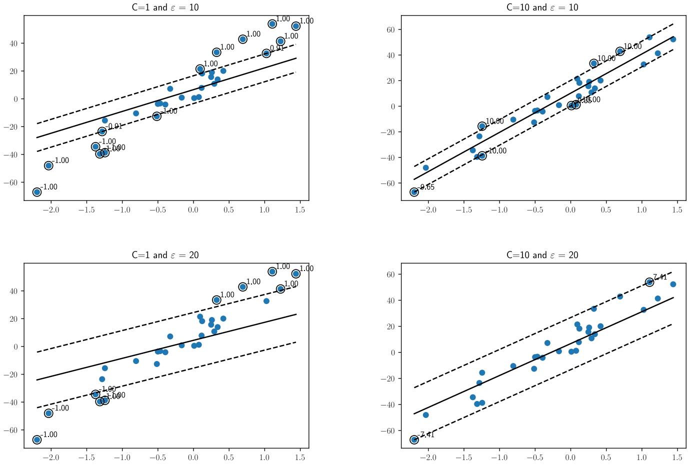
Dual variables

- $\alpha_i, \alpha_i^\star$ for errors constraints
- $\nu_i, \nu_i^\star$ for positivity on $\xi_i^{(\star)}$

Resolution

- $\nu_i^{(\star)} = C - \alpha_i^{(\star)}$
- $\boldsymbol{w} = \sum_{i=1}^N (\alpha_i - \alpha_i^\star)\mathbf{x}_i$
- $f(\mathbf{x}) = \sum_{i=1}^N (\alpha_i - \alpha_i^\star)\mathbf{x}_i^\top \mathbf{x} + b$

C and ε



Others variants of SVM

- Multiclass formulation: $\mathcal{Y} \in \mathbb{N}$
- One class SVM : unsupervised method to detect outliers
- ν-SVM : variant of C-SVM

Let's try it

Let's revisit SVM

Objective function

$$\max_{\alpha} \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^\top \mathbf{x}_j$$

s. t.

$$\alpha_i \geq 0, \forall i \in 1 \ldots N$$

$$\sum_{i=1}^{N} \alpha_i y_i = 0$$

Decision function

$$f(\mathbf{x}') = \boldsymbol{w}^\top \mathbf{x}' + b = \sum_{i=1}^{N} \alpha_i \boldsymbol{y}_i \mathbf{x}_i^\top \mathbf{x}' + b$$

Observations

What does it mean ?

- Decision function is a linear combination of input data
- We don't need explicit data vectors $\mathbf{x}_i$
- We only need values of $\langle \mathbf{x}_i, \mathbf{x}_j \rangle, \forall i, j \in \{1..N\}^2$

Observations

Intuition

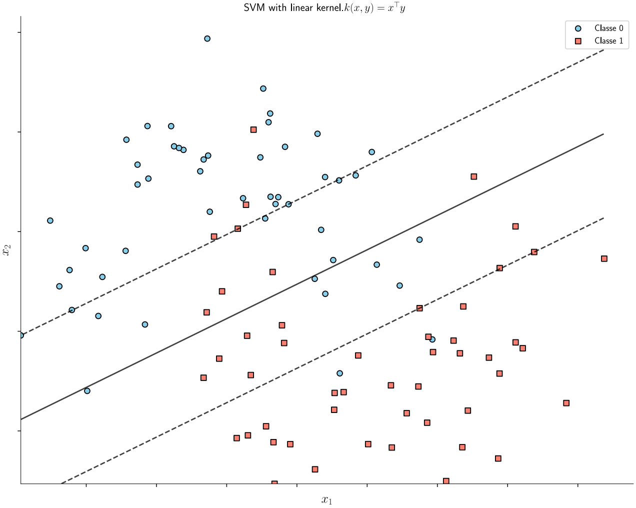
By simply modifying the dot product, the algorithm works in another space

This is the **Kernel Trick**

1. Define your algorithm as it access to data only through scalar products
2. Redefine your scalar product between data by a kernel $k(\cdot, \cdot)$
3. Replace standard scalar product by k
4. Enjoy

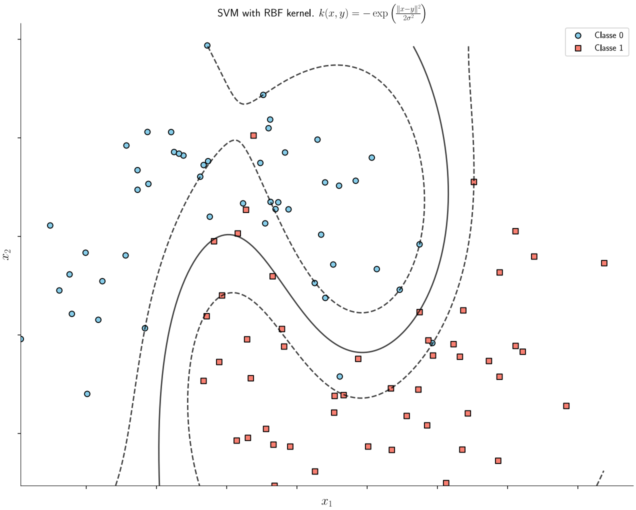
Non linear SVM

Linear SVM



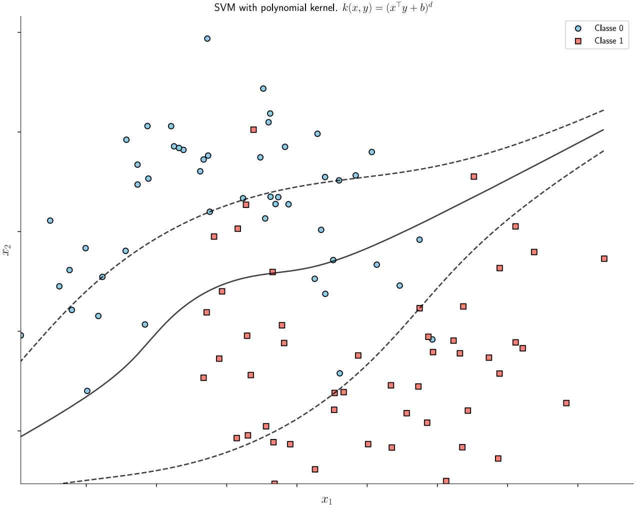
Non linear SVM

Linear SVM



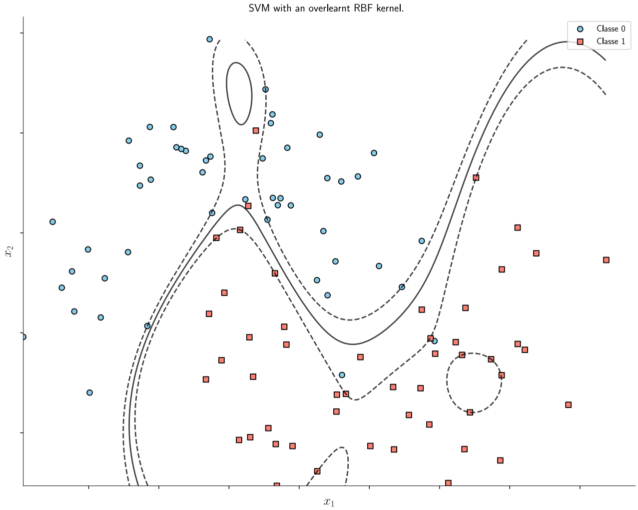
Non linear SVM

Linear SVM



Non linear SVM

Linear SVM



What is a kernel ?

What can be k ?

Prerequisites

Some definitions and notations

- $\mathcal{X}$: Non empty input space (set of $\mathbb{R}^N$, graphs, objects, ...)
- $x \in \mathcal{X}$, $\mathbf{x} \in \mathbb{R}^d$
- $\mathcal{H}$: feature space with a dot product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$
- $\Phi : \mathcal{X} \to \mathcal{H}$: embedding function from $\mathcal{X}$ to $\mathcal{H}$

Kernel

Definition

A kernel k is a function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$:

$$k(x, x') = \langle \Phi(x), \Phi(x') \rangle_{\mathcal{H}}$$

Positive Definite Kernels

Gram Matrix

Given a kernel $k : \mathcal{X}^2 \to \mathbb{R}$, and $\{x_1, \ldots, x_n\} \subseteq \mathcal{X}$, the corresponding Gram Matrix $\mathbf{K}$ is a $n \times n$ matrix whose elements :

$$\mathbf{K}_{i,j} := k(x_i, x_j)$$

Positive Semi-Definite Matrix

- if $\mathbf{K}$ is symmetric and $\mathbf{c}^T\mathbf{K}\mathbf{c} > 0, \forall \mathbf{c} \neq 0$, K is a positive definite matrix
- if $\mathbf{K}$ is symmetric and $\mathbf{c}^T\mathbf{K}\mathbf{c} \geq 0, \forall \mathbf{c} \neq 0$, K is a positive semi-definite matrix.

Equivalently: $\sum_{i=1}^{n} \sum_{j=1}^{n} \mathbf{c}_i \mathbf{c}_j \mathbf{K}_{i,j} \geq 0$

Positive Definite Kernels I

Definition

If for any subset $\mathcal{X}' \subseteq \mathcal{X}, |\mathcal{X}'| = n$, the associated Gram Matrix $\mathbf{K} \in \mathbb{R}^{n \times n}$ is positive semi-definite, then k is a positive definite kernel on $\mathcal{X}$.

- Usually, we talk about kernels. Positiveness is implicit.
- Verifying $\mathbf{K}$ positive semi-definiteness consists in computing eigenvalues $\lambda_1 > \cdots > \lambda_n$. if $\lambda_n \geq 0$, then $\mathbf{K}$ is positive semi-definite.
- Keep in mind that k corresponds to a scalar product in $\mathcal{H}$, so:
  - $k(x_i, x_j) = k(x_j, x_i)$: Then $\mathbf{K}$ is symmetric.
  - Consider $\mathbf{X} \in \mathbb{R}^{n \times d}$, $\mathbf{K} = \mathbf{X}\mathbf{X}^\top$. Eigenvalues > 0 follows.

Reproducing Kernel Hilbert Space

RKHS

- $\mathcal{H}$ is a:
  - pre-Hilbert space of functions
  - endowed with a dot product
  - and we add a norm $\|f\| := \sqrt{\langle f, f \rangle}$
- $\mathcal{H}$ is a Hilbert space.
- Hilbert space: Generalization of euclidean space to finite or infinite dimension

> $\mathcal{H}$ is called a reproducing kernel Hilbert space (RKHS) associated to kernel k

Let's summarize

From kernel to feature space

Given a valid kernel k, we can associate a RKHS $\mathcal{H}$ which corresponds to the feature space of k.

From feature space to kernel

Now consider that you have $\Phi : \mathcal{X} \to \mathcal{H}$ a mapping function.
A positive kernel k is defined by:

$$k(x, x') = \langle \Phi(x), \Phi(x') \rangle_{\mathcal{H}}$$

Kernels in Practice

Linear Kernel

$k(\mathbf{s}, \mathbf{t}) = \mathbf{s}^\top \mathbf{t}$

- $\mathbf{s}, \mathbf{t} \in \mathbb{R}^d$
- symmetric: $\mathbf{s}^\top \mathbf{t} = \mathbf{t}^\top \mathbf{s}$
- positive:

$$\begin{aligned}
\sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j k(\mathbf{x}_i, \mathbf{x}_j) &= \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j \mathbf{x}_i^\top \mathbf{x}_j \\
&= \left(\sum_{i=1}^{n} \alpha_i \mathbf{x}_i \right)^\top \left(\sum_{j=1}^{n} \alpha_j \mathbf{x}_j \right) \\
&= \left\| \sum_{i=1}^{n} \alpha_i x_i \right\|^2
\end{aligned}$$

Product kernel

$k(x, x') = g(x)g(x')$

- $x, x' \in \mathcal{X}$
- for some $g : \mathcal{X} \to \mathbb{R}$
- symmetric: by construction
- positive:

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j k(\mathbf{x}_i, \mathbf{x}_j) = \sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j g(\mathbf{x}_i)g(\mathbf{x}_j)$$

$$= \left(\sum_{i=1}^{n}\alpha_i g(\mathbf{x}_i)\right)\left(\sum_{j=1}^{n}\alpha_j g(\mathbf{x}_j)\right)$$

$$= \left(\sum_{i=1}^{n}\alpha_i g(\mathbf{x}_i)\right)^2$$

Polynomial kernels I

A first approach

- $\mathbf{s}, \mathbf{t} \in \mathbb{R}^N$
- All ordered combinations of degree d, e.g.:

$$\Phi : \mathbb{R}^2 \to \mathcal{H} = \mathbb{R}^4$$
$$(\mathbf{s}_1, \mathbf{s}_2) \mapsto (\mathbf{s}_1^2, \mathbf{s}_2^2, \mathbf{s}_1\mathbf{s}_2, \mathbf{s}_2\mathbf{s}_1)$$

- Dimension of $\mathcal{H}$: $\frac{(d+N-1)!}{d!(N-1)!}$
- Untractable !

Polynomial kernels II

$k(\mathbf{s}, \mathbf{t}) = \langle \mathbf{s}, \mathbf{t} \rangle^d$, $\mathbf{s}, \mathbf{t} \in \mathbb{R}^N$

- Two valid feature spaces:
- All ordered combinations of degree d, e.g.:

$$\begin{aligned} \Phi : \mathbb{R}^2 &\rightarrow \mathcal{H} = \mathbb{R}^4 \\ (\mathbf{s}_1, \mathbf{s}_2) &\mapsto (\mathbf{s}_1^2, \mathbf{s}_2^2, \mathbf{s}_1\mathbf{s}_2, \mathbf{s}_2\mathbf{s}_1) \end{aligned}$$

- All unordered combinations of degree d, e.g.:

$$\begin{aligned} \Phi : \mathbb{R}^2 &\rightarrow \mathcal{H} = \mathbb{R}^3 \\ (\mathbf{s}_1, \mathbf{s}_2) &\mapsto (\mathbf{s}_1^2, \mathbf{s}_2^2, \sqrt{2}\mathbf{s}_1\mathbf{s}_2) \end{aligned}$$

- Also: $(\mathbf{s}^\mathsf{T}\mathbf{t} + c)^d$, $c \in \mathbb{R}^+$.
- High dimensional feature space but k is computed in $\mathcal{O}(n)$

Generalisation: finite kernel

Embedding

- Let Φ_j, for $j = 1, \ldots, p$ be a finite dictionary of functions $\mathcal{X} \to \mathbb{R}$ (polynomials, wavelets, ...)
- Feature map:

$$\begin{aligned} \Phi : \mathcal{X} &\to \mathbb{R}^p \\ \mathbf{s} &\mapsto \big(\Phi_1(x), \ldots, \Phi_p(x')\big) \end{aligned}$$

- Linear kernel in the feature space:

$$k(x, x') = \big(\Phi_1(x), \ldots, \Phi_p(x)\big)^\top \big(\Phi_1(x'), \ldots, \Phi_p(x')\big)$$

Gaussian kernel

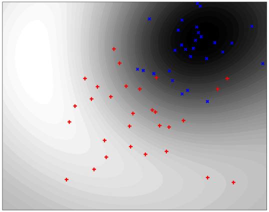
$k(\mathbf{s}, \mathbf{t}) = \exp\left(-\frac{\|\mathbf{s}-\mathbf{t}\|^2}{2\sigma^2}\right)$

- for $\sigma = 1$:

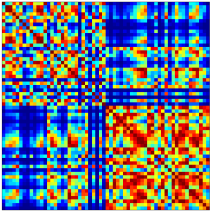
$$\Phi(\mathbf{s}) = \left(\frac{\exp\frac{\|\mathbf{s}\|^2}{2j}}{\sqrt{j!}^{1/j}}\binom{j}{n_1, \ldots, n_k}^{1/2}\mathbf{s}_1^{n_1}\ldots\mathbf{s}_k^{n_k}\right)_{j=0,\ldots,\infty,\sum_{i=1}^k n_i = j}$$

- Feature space has an infinite dimension
- Overlearning ⚠
- σ controls the influence area of the kernel
- σ is another hyperparameter

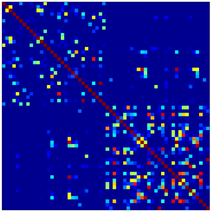
Examples of Gram matrices with different bandwidth



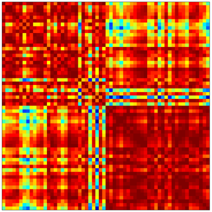
raw data



Gram matrix for $b = 2$



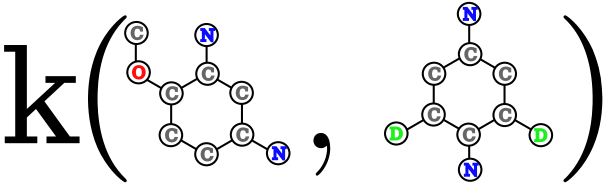
$b = .5$



$b = 10$

Kernels on structures

- $\mathcal{X}$ may not be a vector space.
- we can define kernels on any kind of data :
  - Strings
  - Time series
  - Graphs
  - Images
  - ...



Kernel from distances I

Kernel and distance

- Distance is a dissimilarity measure between vectors or objects

$$
\begin{aligned}
{d_m}^2(\mathbf{s},\mathbf{t}) =& \|\mathbf{s}-\mathbf{t}\|_2^2 \\
=& (\mathbf{s}-\mathbf{t})^\top(\mathbf{s}-\mathbf{t}) \\
=& \mathbf{s}^\top\mathbf{s}+\mathbf{t}^\top\mathbf{t}-2\mathbf{s}^\top\mathbf{t} \\
=& \langle\mathbf{s},\mathbf{s}\rangle+\langle\mathbf{t},\mathbf{t}\rangle-2\langle\mathbf{s},\mathbf{t}\rangle \\
=& k(\mathbf{s},\mathbf{s})+k(\mathbf{t},\mathbf{t})-2\,k(\mathbf{s},\mathbf{t})
\end{aligned}
$$

- For normalized kernels ($k(x,x')=1$) kernel is proportional to the opposite of squared distance
- Kernels correspond to similarity measures

Kernel from distances II

From distance to kernels

- We can define a kernel from an euclidean distance
- Usually we plug a distance in Gaussian Kernel
- Use of distance map

$$\mathcal{X} \rightarrow \mathbb{R}^n$$
$$\Phi(x) = (d_m(x, x_1), \ldots, d_m(x, x_n))$$

- Related to kernel feature map

Kernel jungle

Appendix D

List of kernels

D.1 Kernel definitions and computations

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D.2 Kernel algorithms

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[Shawe-Taylor and Cristianini, 2004]

Invalid kernels

Danger

Some similarity measures may be invalid kernels

- $k(x, y) = \max(x, y)$.
- Optimal assignment kernel: [Fröhlich et al., 2005]
- and many more ...
- The use is not forbidden, but handle with care
- $\rightarrow$ operating in Krein spaces: [Loosli et al., 2013]

Kernel algebra

Convex cone:

The set of kernels forms a convex cone, closed under pointwise convergence.

- **Linear combination**:
  - if k_1 an k_2 are kernels, a_1,$a_2 \geq 0$, then $a_1 k_1 + a_2 k_2$ is a kernel
  - if k_1, k_2, ...are kernels, and $k(x, x') := \lim_{n \to \infty} k_n(x, x')$ exists for all x, x', then k is a kernel
- **Product kernel**:
  if k_1 an k_2 are kernels, then $k_1 k_2(x, x') := k_1(x, x') k_2(x, x')$ is a kernel.

And some molecular graphs kernels

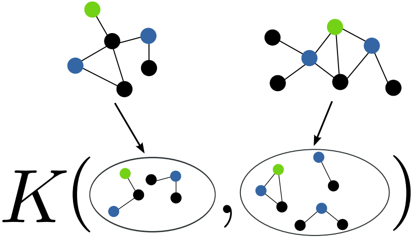
How to define the similarity between molecules ?

Graph kernel based on bags of patterns

(1) Extraction of a set of patterns,

(2) Comparison between patterns,

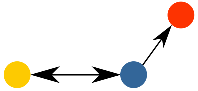
(3) Comparison between bags of patterns.

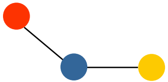


Patterns

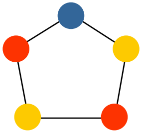
Linear Patterns

- **Random Walks** ∞ **Kashima et al. [2003]**
  - − Tottering
  - \+ Mahé et al. [2004b].





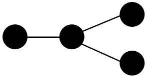
- **Paths** $\not\infty$ **Ralaivola et al. [2005]**
  - − Low branching description

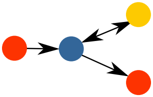


- **Cyclic patterns** $\not\infty$ **Horváth et al. [2004]**
  - \+ Cyclic information
  - \+ Relevant in chemoinformatics
  - − Only a partial cyclic information

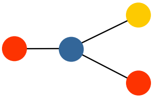
Patterns

- **Graphlets** $\not\propto$ **Shervashidze et al. [2009]**
  - ✚ Non linear structures.
  - ▬ Non labeled patterns.
  - ✚ Linear complexity.





- **Tree-patterns** $\propto$ **Mahé and Vert [2009], ?**
  - ✚ Non linear and labeled patterns.



- **Treelets** $\not\propto$ **Gaüzère et al. [2012b]**
  - ✚ Non linear and labeled patterns.

Convolution Kernels

Counting function

- $f_p(G)$: Number of occurences of pattern p in G.

Kernel definition

$$k_{\mathcal{T}}(G, G') = \sum_{p \in \mathcal{P}(G) \cap \mathcal{P}(G')} k_p(G, G')$$

- $\mathcal{P}(G)$: Set of patterns extracted from G.
- $k_p(G, G') = k(f_p(G), f_p(G'))$.
- $k_p(.,.)$: Similarity according to p.

Molecular similarity

$\Longleftrightarrow$

Similarity of their bags of patterns

Conclusion

SVM

- Nice framework
- Good mathematical foundations
- Kernel trick : extension to non linear models and any data

Limitations

- Need to define and compute a kernel
- Still need to handcraft features (or kernel)

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