Lab SVM

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This lab aims at introducing SVM and use them on real and synthetic datas using the package scikit-learn. We first recall some definitions and notations

1 Introduction and theoritical background

- We denote \mathcal{Y} the labels. Usually $\mathcal{Y} = \{-1, +1\}$
- $x = (x_1, \dots, x_p) \in \mathcal{X} \subset \mathbb{R}^p$ is an observation
- $Dn = \{(x_i, y_i), i = 1, \dots, n\}$ a training set containing n examples and their labels
- We assume that there exists a probabilistic model explaining the generation of the datas from random variables X and Y:

$$\forall i \in \{1, \cdots, n\}, (x_i, y_i) \stackrel{(i.i.d.)}{\sim} (X, Y)$$

• We aim at defining from the training set \mathcal{D}_n a function $\hat{f}: \mathcal{X} \to \{-1,1\}$ predicting for any new point x its label. Here the decision rule will be linear, that is we separate the space by an hyperplane and we predict -1 or 1 according to the position of x with respect to this hyperplane.

SVM and kernel for binary classification

Non linear SVM involve an implicit function Φ transforming the input space $\mathcal{X} \subset \mathbb{R}^p$ into an Hilbert space $(\mathcal{H}, < ., . >$ whose dimension is greater. Learning is done from the model $(\Phi(X), Y)$ in \mathcal{H} . What is expected is that in this new feature space, the data become more linearly separable. From the practical point of view let us observe that one does not compute the projections of $\Phi(X)$. We only use the scalar products $<\Phi(X), \Phi(X')>$. These scalar products can be computed using a kernel (kernel trick)

$$K(x,x') = <\Phi(x), \Phi(x')>$$

We need to choose carefully a kernel, usual choices are the following

- Linear kernel : $K(x, x') = \langle x, x' \rangle$ (corresponding to linear SVM)
- Radial Gaussian kernel (Gaussian RBF)

$$K(x, x') = \exp(-\gamma ||x - x'||^2)$$

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- Polynomial kernels $K(x, x') = (\alpha + \beta < x, x' >)^{\delta}$
- Laplace radial kernel $K(x, x') = \exp(-\gamma ||x x'||)$
- Sigmoide kernel $K(x, x') = tanh(\alpha + \beta < x, x' >)$

A SVM classifier is of the form

$$\widehat{f}_{w,w_0}(x) = sign(\langle w, \Phi(x) \rangle + w_0)$$

where $w \in \mathcal{H}, w_0 \in \mathbb{R}$ are parameters learning from the training set $\mathcal{D}_n = \{(x_i, y_i), i \in \{1, \dots, n\}\}$. The boundary associated to this decsion rule is the set $\{x, < w, \Phi(x) > +w_0 = 0\}$. This et corresponds to an hyperplane in \mathcal{H} but is much more complex in \mathcal{X} . In \mathcal{H} , we obtain the separating hyperplane maximizing the margin separating the two classes, that is solving the following optimization problem:

$$\begin{cases} (w^*, w_0^*, \xi^*) \in \operatorname{argmin}_{w \in \mathcal{H}, w_0 \in \mathbb{R}, \xi \in \mathbb{R}^n} \left(\frac{1}{2} ||w||^2 + C \sum_{i=1}^n \xi_i \right) \\ \text{s.c. } \xi_i \ge 0 \\ y_i(< w, \Phi(x_i) > +w_0) \ge 1 - \xi_i \end{cases}$$

The solution w of this problem is of the form

$$w = \sum_{i=1}^{n} \alpha_i^* y_i \Phi(x_i)$$

The coefficients α_i^* are solutions of the dual problem

$$\begin{cases} \alpha^* \in \operatorname{argmax}_{\alpha \in \mathbb{R}^n} \left(\sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{1 \le i, j \le n} \alpha_i \alpha_j y_i y_j K(x_i, x_j) \right) \\ \text{s.c. } 0 \le \alpha \le C, \forall i \in \{1, \cdots, n\} \\ \sum_{i=1}^n \alpha_i y_i = 0 \end{cases}$$

The parameter C is related to the complexity of the classifier. More precisely, it measures the cost of a misclassification. The larger is C, the more complex is the decision rule. This approach is called the C classification. One uses the object sklearn.sym.SVC in scikit-learn. Another approach consists in considering the following alternative problem:

$$\begin{cases} \alpha^* \in \operatorname{argmax}_{\alpha \in \mathbb{R}^n} \left(\sum_{1 \leq i, j \leq n} \alpha_i \alpha_j y_i y_j K(x_i, x_j) \right) \\ \text{s.c. } 0 \leq \alpha \leq 1, \forall i \in \{1, \dots, n\} \\ \sum_{i=1}^n \alpha_i y_i = 0 \sum_{i=1}^n \alpha_i \geq \nu \end{cases}$$

where $\nu \in [0,1]$. This approach is used with the object sklearn.svm.NuSVC of the package scikit-learn.

Extensions to the multiclass setting

In the case where the output variable Y can take more than two values there is several ways to extend the methods of the binary case

- "One against one" In the case where we want to predict a label taking more than two values one can consider all the possible pairs of label (k, l) and fit a classifier $C_{k, l}$ for each one. One then predicts the label who won most of the comparisons
- "One against all" For each possible value of the output variable, we learn a classifier allowing to discriminate between the two populations Y = k and $Y \neq k$. Using the a posteriori probabilities, one affects the most probable label.

2 SVM in practice

We shall use the object sklearn.svm.SVC: from sklearn.svm import SVC

1. Use the website:

http://scikit-learn.org/stable/modules/svm.html

and the dataset Iris. Implement a classifier which classifies class 1 against class 2 of the dataset iris using the two first variabme and a linear kernel. Use half of the dataset for training and half of the dataset for validation. To import the dataset iris, type

from sklearn import datasets
iris = datasets.load_iris()

X = iris.data

y = iris.target

X = X[y != 0, :2]

y = y[y != 0]

- 2. Compare the result with a SVM based on polynomial kernel
- 3. Prove that the primal problem can also be reformulated as follows

$$\operatorname{argmin}_{w \in \mathcal{H}, w_0 \in \mathbb{R}} \frac{1}{2} ||w||^2 + C \sum_{i=1}^n [1 - y_i(\langle w, \Phi(x_i) \rangle + w_0)]_+$$

- 4. Use the script svm_gui.py. This application allows to evaluate the impact of the choice of the kernel and the regularisation parameter C.
- 5. Generate a dataset with much more observations in one class than another (for e.g. 90% vs 10%).
- 6. Use a linear kernel and decrease the parameter C. Comment