Hyper-parameters auto-setting using regularization path for ν-SVM

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Abstract

- Goal: auto-setting of the regularization parameter for SVM
- Tools:
  - Simple-ν-SVM solver
  - Regularization path for SVM
  - Leave-one-out validation method

ν-SVM

We consider a binary classification problem with training patterns $x_1 \dots x_m \in \mathcal{X}$ and classes $y_1 \dots y_m \in \{+1, -1\}$.

$$\begin{cases} \min_{f,b,\rho,\xi_i} \frac{m}{2}\|f\|^2 - \lambda\rho + \sum_{i=1}^{m} \xi_i \\ \text{s.t. } y_i\big(f(x_i)+b\big) \geq \rho - \xi_i & \forall i \in [1,\dots,m] \\ \text{and } \rho \geq 0 \\ \text{and } \xi_i \geq 0 & \forall i \in [1,\dots,m] \end{cases}$$

$$\begin{cases} \max_{\alpha} -\frac{1}{2}\boldsymbol{\alpha}^\top G \boldsymbol{\alpha} \\ \text{s.t. } \boldsymbol{\alpha}^\top \mathbf{1} \geq \lambda \\ \text{and } \boldsymbol{\alpha}^\top \mathbf{y} = 0 \\ \text{and } 0 \leq \alpha_i \leq 1 & \forall i \in [1,\dots,m] \end{cases}$$

where $G(i,j) = \frac{1}{m} y_i y_j k(x_i, x_j)$.

Regularization path

Our aim is to compute the ν-SVM solution for all values of ν. As shown in [1], the path is piecewise linear. It means that the support vectors set does not change between two values of ν. Hence we only need to identify when a change occurs in the sets.

Let note $g(x_i) = y_i\big(f(x_i)+b\big) - \rho$. Then we have:

$$\begin{cases} \mathcal{L} : g(x_i) < 0 \; \forall i \in \mathcal{L} & \alpha_i = 1 & \text{bounded points} \\ \mathcal{E} : g(x_i) = 0 \; \forall i \in \mathcal{E} & 0 < \alpha_i < 1 & \text{margins points} \\ \mathcal{R} : g(x_i) > 0 \; \forall i \in \mathcal{R} & \alpha_i = 0 & \text{useless points} \end{cases}$$

We identify four possible movements:

Step	$in(r)$	$out(r)$	$out(\ell)$	$in(\ell)$
t	$i \in \mathcal{R}$	$i \in \mathcal{E}$	$i \in \mathcal{E}$	$i \in \mathcal{L}$
	$g^t(x_i) > 0$	$\star\mathbf{g^t(x_i) = 0}$	$\star\mathbf{g^t(x_i) = 0}$	$g^t(x_i) < 0$
verte	$\alpha_i = 0$	$0 < \alpha_i < 1$	$0 < \alpha_i < 1$	$\alpha_i = 1$
$t+1$	$i \in \mathcal{E}$	$i \in \mathcal{R}$	$i \in \mathcal{L}$	$i \in \mathcal{E}$
	$\star\mathbf{g^{t+1}(x_i) = 0}$	$\star\mathbf{g^{t+1}(x_i) \geq 0}$	$\star\mathbf{g^{t+1}(x_i) \leq 0}$	$\star\mathbf{g^{t+1}(x_i) = 0}$
	$0 < \alpha_i < 1$	$\star\mathbf{\alpha_i = 0}$	$\star\mathbf{\alpha_i = 1}$	$0 < \alpha_i < 1$

Summary of the events. Each column stands for a particular event. In blue starred are noted the properties that are used to compute the corresponding λ^{t+1}

The Simple-ν-SVM solver

The Simple-ν-SVM solver is derived from the SimpleSVM [2]. It is an active set method, based on the repartition of the training points into three groups :

- $\mathcal{R}$ for unused points,
- $\mathcal{E}$ for support vectors placed on the margins,
- $\mathcal{L}$ for support vectors placed further.

Algorithm:

```
initialisation, ν = 1/n
while ν < 1 do
    solve linear system                              ▷ α_w
    if non admissible solution then
        project solution in the admissible set       ▷ Simple-ν-SVM step
    else if non optimal solution then
        select next point                            ▷ Simple-ν-SV step
    else
        compute the next ν                           ▷ regularization path step
    end if
end while
```

Stopping criteria

The leave-one-out error is defined as the mean error done for the removed points. We also compute a second leave-one-out estimation to have an idea of the variance of the solution:

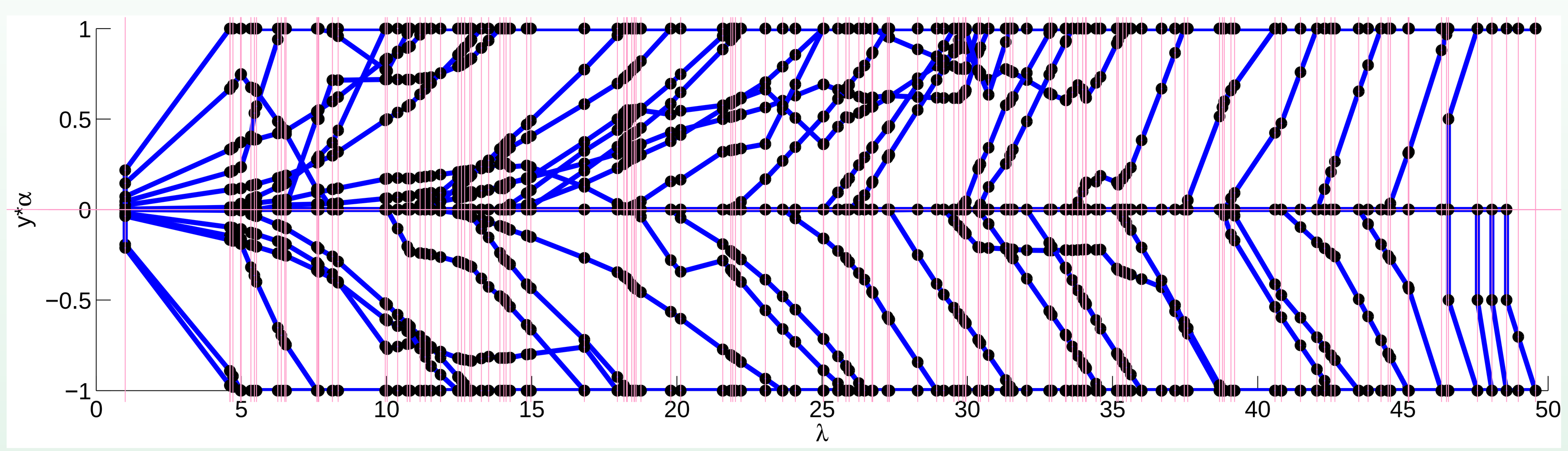
$$LOO1_{error} = \frac{1}{n}\sum_i 1 - sign(\hat{y}_i y_i) \qquad LOO2_{error} = \frac{1}{n}\sum_i max(0, \rho - \hat{y}_i y_i)$$

This second formula is very helpful to detect over-fitting. Indeed, outliers will be very penalized.

- leave-one-out error rates are estimated at each step,
- no point from $\mathcal{R}$ participate to the solution $\rightarrow$ zero error,
- need to compute the LOO errors of each point of $\mathcal{E}$ and $\mathcal{L}$ only,
- Simple-ν-SVM warm start.

Experiments

For the evaluation of our method, we have used the artificial *apple and banana* dataset.



Evaluation of the $y_i\alpha_i$ along the path for the apple and banana problem. The regularization paths can be represented via the values taken by the α coefficients during learning. Those coefficients follow piecewise linear paths. $\alpha_i y_i$ is plot, such that all negative points appear bellow zeros.

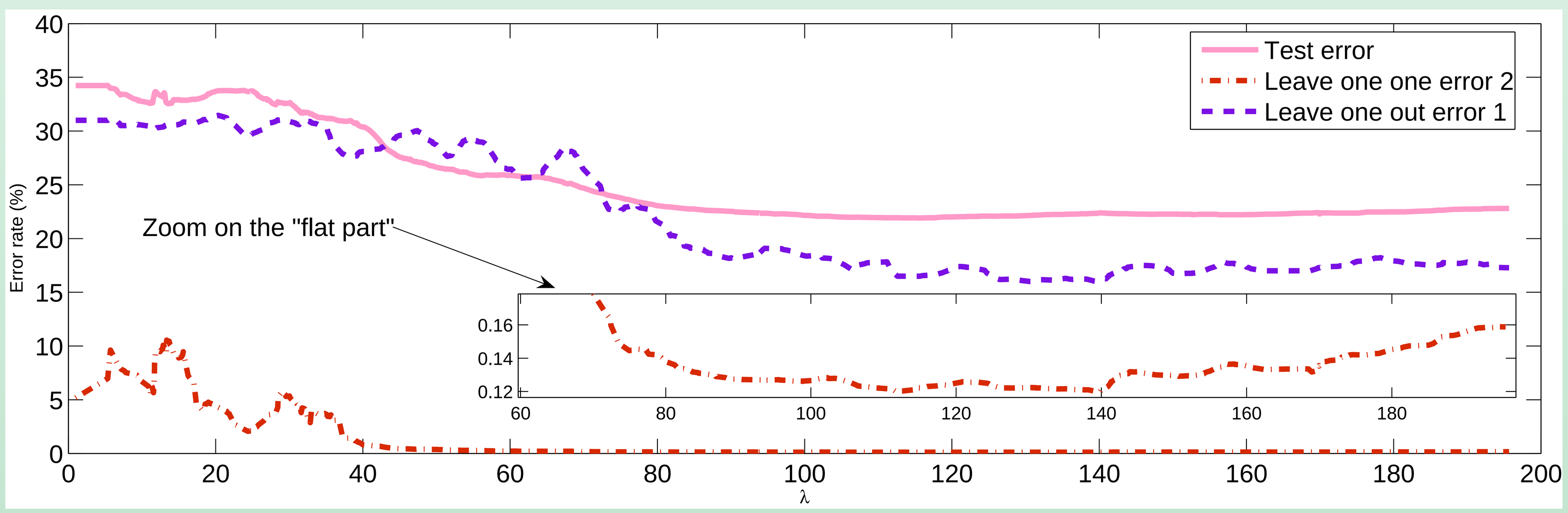


Illustration on the apple en banana dataset of the LOO error rate evolution according to λ, reported with the test error.

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References

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Conclusion

- ν-SVM regularization path
- stopping criteria to auto-set the regularzation parameter
- efficient ν-SVM solver
- method taking advantage of the sparcity
- allow to use regularization paths for larger databases