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Embedded Variable Selection in Classification Trees

Servane Gey¹, Tristan Mary-Huard²

¹MAP5, UMR 8145, Université Paris Descartes, Paris, France

²UMR AgroParisTech/INRA 518, Paris, France



Introduction

- ★ Binary classification setting
- ★ Model and variable selection in classification
- ★ Classification tree

Variable selection for CART

- ★ Classes of classification trees
- ★ Theoretical results
- ★ Comparison with practice.

Binary classification

Binary classification

Prediction of the unknown label Y (0 or 1) of an observation X .

⇒ Use training sample $D = (X_1, Y_1), \dots, (X_n, Y_n) \stackrel{i.i.d}{\sim} \mathbb{P}$ to build a classifier \hat{f}

$$\begin{aligned}\hat{f}: \mathcal{X} &\rightarrow \{0, 1\} \\ X &\mapsto \hat{Y}.\end{aligned}$$

Quality assessment

★ Classification risk and loss : Quality of the resulting classifier \hat{f}

$$\begin{aligned}L(\hat{f}) &= \mathbb{P}(\hat{f}(X) \neq Y|D) \\ \ell(\hat{f}, f^*) &= L(\hat{f}) - L(f^*)\end{aligned}$$

★ Average loss : Quality of the classification algorithm

$$\mathbb{E}_D[\ell(\hat{f}, f^*)]$$

Remark : All these quantities depend on \mathbb{P} that is unknown.

Basics of Vapnik Theory : structural risk minimization (SRM)

Consider and collection of classes of classifiers $\mathcal{C}_1, \dots, \mathcal{C}_M$. Define

$$\bar{f}_m = \arg \min_{f \in \mathcal{C}_m} L(f), \quad \hat{f}_m = \arg \min_{f \in \mathcal{C}_m} L_n(f), \quad \hat{f} = \arg \min_m \left[L_n(\hat{f}_m) + \alpha \frac{V_{\mathcal{C}_m}}{n} \right]$$

★ Class complexity

If $\mathcal{C}_1, \dots, \mathcal{C}_M$ have finite VC dimensions $V_{\mathcal{C}_1}, \dots, V_{\mathcal{C}_M}$, then

$$\mathbb{E}_D [\ell(\hat{f}, f^*)] \leq C \left\{ \inf_m \left(\ell(\bar{f}_m, f^*) + K \sqrt{\frac{V_{\mathcal{C}_m}}{n}} \right) \right\} + \frac{\lambda}{n} \quad (\text{Vapnik, 1998}).$$

★ Classification task complexity (Margin Assumption)

If there exists $h \in]0; 0.5[$ such that

$$\mathbb{P} (|\eta(x) - 1/2| \leq h) = 0, \quad \text{with } \eta(x) = \mathbb{P}(Y = 1 | X = x)$$

then

$$\mathbb{E}_D [\ell(\hat{f}, f^*)] \leq C \left\{ \inf_m \left(\ell(\bar{f}_m, f^*) + K' \left(\frac{V_{\mathcal{C}_m}}{n} \right) \right) \right\} + \frac{\lambda'}{n} \quad (\text{Massart \& Nédélec, 2006}).$$

Assume that $X \in \mathbb{R}^p$. Define

$$\bar{f}_{m(k)} = \arg \min_{f \in \mathcal{C}_{m(k)}} L(f), \quad \hat{f}_{m(k)} = \arg \min_{f \in \mathcal{C}_{m(k)}} L_n(f)$$

★ Variable selection

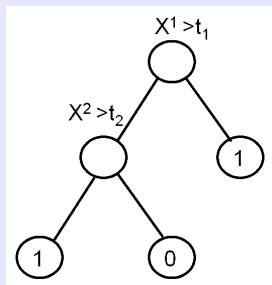
Choose \hat{f} such that

$$\hat{f} = \arg \min_{m(k)} \left[L_n(\hat{f}_{m(k)}) + \alpha \frac{V_{\mathcal{C}_{m(k)}}}{n} + \alpha' \log \binom{p}{k} \right]$$

Then (under strong margin assumption)

$$\mathbb{E}_D [\ell(\hat{f}, f^*)] \leq C \log(p) \left\{ \inf_{m(k)} \left(\ell(\bar{f}_{m(k)}, f^*) + K' \left(\frac{V_{\mathcal{C}_{m(k)}}}{n} \right) \right) \right\} + \frac{\lambda}{n}$$

(Massart, 2000, Mary-Huard et al., 2007)



General strategy

Choose

$$\hat{f} = \arg \min_T L_n(f_T) + \alpha \frac{|T|}{n}$$

Heuristic approach (CART, Breiman, 1984)

★ Find a tree T_{\max} such that $L_n(f_{T_{\max}}) = 0$,

★ Prune T_{\max} using criterion :

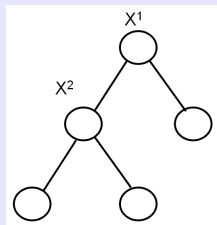
$$\hat{f} = \arg \min_{T \subseteq T_{\max}} L_n(f_T) + \alpha \frac{|T|}{n}$$

Definitions

Consider a tree T_{cl} with

- a given configuration c ,
- a given list ℓ of associated variables.

Remark : A same variable may be associated with several nodes.



Class of tree classifiers

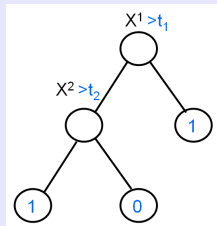
Define

$$\mathcal{C}_{cl} = \{f/f \text{ based on } T_{cl}\},$$

$$H_{cl} = \text{VC log-entropy of class } \mathcal{C}_{cl},$$

$$\bar{f}_{cl} = \underset{f \in \mathcal{C}_{cl}}{\operatorname{argmin}} L(f),$$

$$\hat{f}_{cl} = \underset{f \in \mathcal{C}_{cl}}{\operatorname{argmin}} L_n(f).$$



Remark : Two classifiers $f, f' \in \mathcal{C}_{cl}$ only differ in their thresholds and labels.

Proposition

Assume that strong margin assumption is satisfied. For all $C > 1$, there exist positive constants K^1 and K^2 depending on C such that

$$\mathbb{E}_D[\ell(\widehat{f}_{cl}, f^*)] \leq C \left\{ \ell(\bar{f}_{cl}, f^*) + K^1 \left(\frac{|T_{cl}| \log(2n)}{n} \right) \right\} + \frac{K^2}{n} .$$

Idea of proof

- ★ Show that $E[H_{cl}] \leq |T_{cl}| \log(2n)$,
- ★ Apply general theory (Koltchinskii, 2006).

To take into account variable selection in the penalized criterion, one needs to count the number of classes sharing the same a priori complexity.

★ **Parametric case** (Logistic regression, LDA,...)

- One parameter per variable,
- 2 classes with classifiers based on k variables have the same a priori complexity,
⇒ $\binom{p}{k}$ classes of a priori complexity k .

★ **Classification trees**

- One parameter per internal node (threshold),
- 2 classes \mathcal{C}_{cl} and $\mathcal{C}_{c'l'}$ such that $|T_{cl}| = |T_{c'l'}|$ have the same a priori complexity
⇒ **Count the number of classes based on trees of size k !**

Combinatorics for variable selection

A tree $T_{c\ell}$ is defined by

- a configuration,
- a list of variables associated with each node.

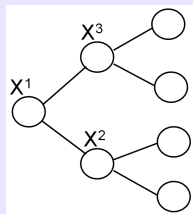
★ Number of configurations of size k :

$$N_c^k = \frac{1}{k} \binom{2k-2}{k-1}$$

★ Number of variable lists of size k :

- the list is ordered : $\{1, 2, 3\} \neq \{2, 1, 3\}$,
- variables are selected with replacement : $\{1, 2, 1\}$.

$$\Rightarrow N_\ell^k = p^{k-1} \text{ instead of } \binom{p}{k} !$$



★ Number of classes based on trees of size $|T_{c\ell}| = k$:

$$N^k = N_c^k \times N_\ell^k = \frac{1}{k} \binom{2k-2}{k-1} \times p^{k-1}$$

$$\Rightarrow \log(N^k) \leq \lambda |T_{c\ell}| \log(p)$$

Combinatorics for variable selection

A tree T_{cl} is defined by

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- a list of variables associated with each node.

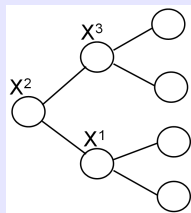
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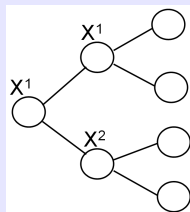
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★ Number of classes based on trees of size $|T_{cl}| = k$:

$$N^k = N_c^k \times N_\ell^k = \frac{1}{k} \binom{2k-2}{k-1} \times p^{k-1}$$

$$\Rightarrow \log(N^k) \leq \lambda |T_{cl}| \log(p)$$

Proposition

Assume that strong margin assumption is satisfied. If

$$\hat{f} = \arg \min_{c, \ell} (L_n(\hat{f}_{c\ell}) + \text{pen}(c, \ell)),$$
$$\text{where } \text{pen}(c, \ell) = C_h^1 \frac{|T_{c\ell}| \log(2n)}{n} + C_h^2 \frac{|T_{c\ell}| \log(\rho)}{n}$$

with constants C_h^1, C_h^2 depending on h appearing in the margin condition, then there exist positive constants C, C', C'' such that

$$\mathbb{E}_D[l(\hat{f}, f^*)] \leq C \log(\rho) \left\{ \inf_{c, \ell} \left\{ \ell(\bar{f}_{c\ell}, f^*) + C' \left(\frac{|T_{c\ell}| \log(2n)}{n} \right) \right\} \right\} + \frac{C''}{n}.$$

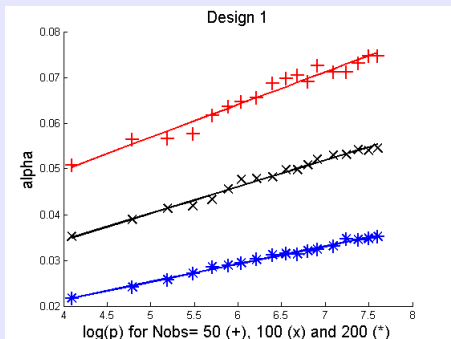
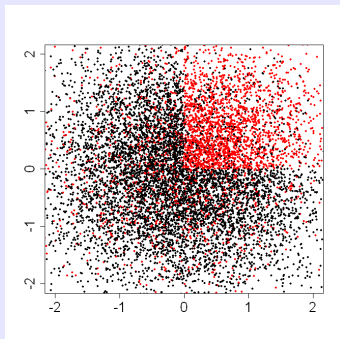
Remark :

$$\text{Theory : } \text{pen}(c, \ell) = (a_n + b_n \log(\rho)) |T_{c\ell}| = \alpha_{p,n} |T_{c\ell}|$$

$$\text{Practice (CART) : } \text{pen}(c, \ell) = \alpha_{CV} |T_{c\ell}|$$

Does α_{CV} match $\alpha_{p,n}$?

Illustration on simulated data (1)

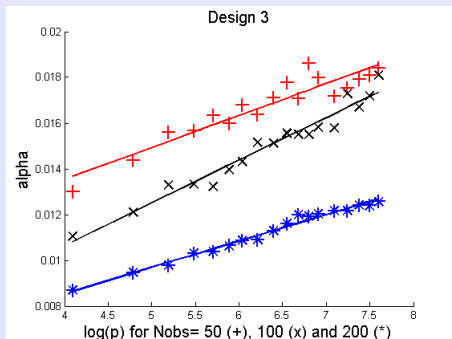
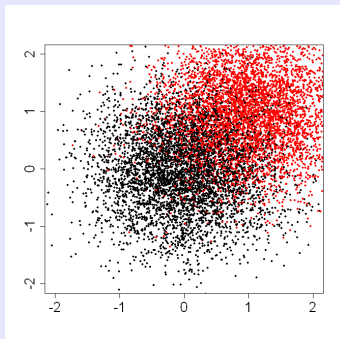


- Variables X^1, \dots, X^p are independent,
- If $X^1 > 0$ and $X^2 > 0$ $P(Y = 1) = q$, otherwise $P(Y = 1) = 1 - q$

Remark : Easy case

- The Bayes classifier belongs to the collection of classes,
- Strong margin assumption is satisfied.

Illustration on simulated data (2)



- $P(Y = 1) = 0.5$
- For $j = 1, 2$, $X^j | Y = 0 \hookrightarrow \mathcal{N}(0, \sigma^2)$ and $X^j | Y = 1 \hookrightarrow \mathcal{N}(1, \sigma^2)$,
- Additional variables are independent and non-informative.

Remark : Difficult case

- The Bayes classifier does NOT belong to the collection of classes,
- Strong margin assumption is NOT satisfied.

Model selection for tree classifiers :

- Already investigated (Nobel 02, Gey & Nedelec 06, Gey 10),
- Variable selection not investigated so far.
- Pruning step now validated from this point of view.

Theory vs practice

- Theory : exhaustive search,
- Practice : forward strategy,
- Nonetheless theoretical results are informative !

Extension

- In this talk : strong margin assumption
- Can be extended to less restrictive margin assumption
- Manuscript on arXiv.org :

<http://arxiv.org/abs/1108.0757>

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