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Embedded Variable Selection in Classification Trees

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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

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

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

$$
\hat{f} : \mathcal{X} \rightarrow \{0, 1\}
$$

$X \mapsto \hat{Y}$.

Quality assessment

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

$$
L(\hat{f}) = \mathbb{P}(\hat{f}(X) \neq Y | D)
$$

$$
\ell(\hat{f}, f^*) = L(\hat{f}) - L(f^*)
$$

★ 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.
Consider a collection of classes of classifiers $\mathcal{C}_1, \ldots, \mathcal{C}_M$. Define

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

★ Class complexity

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

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

★ Classification task complexity (Margin Assumption)

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

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

then

$$\mathbb{E}_D[\ell(\hat{f}, f^*)] \leq C \left\{ \inf_m \left( \ell(\tilde{f}_m, f^*) + K' \left( \frac{\mathcal{VC}_m}{n} \right) \right) \right\} + \frac{\lambda'}{n} \quad \text{(Massart & Nédélec, 2006).}$$
Assume that $\mathbf{X} \in \mathbb{R}^p$. Define

$$\overline{f}_{m(k)} = \arg \min_{f \in C_{m(k)}} L(f), \quad \hat{f}_{m(k)} = \arg \min_{f \in C_{m(k)}} L_n(f)$$

★ Variable selection

Choose $\hat{f}$ such that

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

Then (under strong margin assumption)

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

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

General strategy

Choose

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

Heuristic approach (CART, Breiman, 1984)

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

★ Prune \( T_{\text{max}} \) using criterion :

\[ \hat{f} = \arg \min_{T \subseteq T_{\text{max}}} L_n(f_T) + \alpha \frac{|T|}{n} \]
Consider a tree $T_{c\ell}$ with
- a given configuration $c$,
- a given list $\ell$ of associated variables.

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

**Class of tree classifiers**

Define

$$C_{c\ell} = \{ f / f \text{ based on } T_{c\ell} \}$$

$$H_{c\ell} = \text{VC log-entropy of class } C_{c\ell},$$

$$\bar{f}_{c\ell} = \arg\min_{f \in C_{c\ell}} L(f),$$

$$\hat{f}_{c\ell} = \arg\min_{f \in C_{c\ell}} L_n(f).$$

**Remark:** Two classifiers $f, f' \in C_{c\ell}$ 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

$$
E_D[\ell(\hat{f}_{c\ell}, f^*)] \leq C \left\{ \ell(f_{c\ell}, f^*) + K^1 \left( \frac{|T_{c\ell}| \log(2n)}{n} \right) \right\} + \frac{K^2}{n}.
$$

Idea of proof

★ Show that $E[H_{c\ell}] \leq |T_{c\ell}| \log(2n)$,
★ 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,
  \[ \Rightarrow \binom{p}{k} \text{ classes of a priori complexity } k. \]

★ **Classification trees**
- One parameter per internal node (threshold),
- 2 classes $C_{c\ell}$ and $C_{c'\ell'}$ such that $|T_{c\ell}| = |T_{c'\ell'}|$ have the same a priori complexity
  \[ \Rightarrow \text{Count the number of classes based on trees of size } k! \]
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: $\{1, 2, 1\}$.

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

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

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

$$\Rightarrow \log(N^k) \leq \lambda |T_{c\ell}| \log(p)$$
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: $\{1, 2, 1\}$.
  \[ \Rightarrow N_\ell^k = p^{k-1} \] 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 $T_{c\ell}$ 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 : $\{1, 2, 1\}$.

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

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

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

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

Assume that strong margin assumption is satisfied. If

\[ \hat{f} = \arg\min_{c, \ell} \left( L_n(\hat{f}_{c\ell}) + \text{pen}(c, \ell) \right), \]

where

\[ \text{pen}(c, \ell) = C_h^1 \frac{|T_{c\ell}| \log(2n)}{n} + C_h^2 \frac{|T_{c\ell}| \log(p)}{n} \]

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

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

Remark:

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

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

Does \( \alpha_{CV} \) match \( \alpha_{p,n} \)?
- Variables $X^1, \ldots, X^p$ 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 $j = 1, 2$, $X^j | Y = 0 \sim \mathcal{N}(0, \sigma^2)$ and $X^j | Y = 1 \sim \mathcal{N}(1, \sigma^2)$,
- 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:
  \[ http://arxiv.org/abs/1108.0757 \]


