▲ロト ▲帰ト ▲ヨト ▲ヨト 三日 - の々ぐ

Imprecise Extensions of Random Forests and Random Survival Forests

Lev V. Utkin, Maxim Kovalev, Anna Meldo, Frank Coolen

ISIPTA, Gent, July 2019

Authors are from ...

- Peter the Great St.Petersburg Polytechnic University
- Saint-Petersburg Clinical Research Center for Special Types of Medical Care (Oncological)
- Ourham University



Lev Utkin



Maxim Kovalev



Anna Meldo



Frank Coolen

Classification problem statement

- Given N training examples $S = \{(\mathbf{x}_1, y_1), ..., (\mathbf{x}_N, y_N)\}, \mathbf{x}_i \in \mathbb{R}^m, y_i \in \{1, ..., C\}$
- We aim to construct an accurate classifier c : $\mathbb{R}^m \to \{1, ..., C\}$
- An ensemble-based classifier is the Random Forest (RF)

Random Forest



- Class probabilities are defined by numbers of training examples which fall into leaf nodes
- The class probabilities of the RF are computed by averaging probabilities of trees

・ロト ・ 厚 ト ・ ヨ ト ・ ヨ ト

Weighted Random Forest

• Weights of trees and weighted averaging



Obstacles:

- The number of training examples which fall into a leaf node may be very small
- Precise class probabilities cannot be expected

Two ways for solving the problem

- The first way is to change splitting rules for tree building (Abellan et al. 2017, Abellan et al., Mantas-Abellan, 2014)
 - it leads to changing a tree building algorithm
 - it cannot be directly applied to regression or survival analysis
- The second way is to train a meta-learner which takes into account imprecision of the class probabilities

Meta-learner: Underlying ideas

- the meta-learner produces weights of trees or corresponding class probabilities
- imprecision of the tree estimates (class probabilities) is defined by an imprecise statistical inference model, for example, the IDM
- or robust (pessimistic or maximin) strategy should be applied to the meta-learner
- special loss functions should be proposed to simplify optimization problems for computing optimal weights

An example of the whole classifier



◆□▶ ◆□▶ ◆三▶ ◆三▶ 三三 のへぐ

Loss function

- Weights are taken
 - to minimize Euclidean distance between a training class vector and the obtained class probabilities
 - e to maximize the distance over "imprecise" sets of tree class probabilities
- A standard way for constructing maximin optimization problem:

$$\max_{\mathbf{P}(i,t)\in\mathcal{P}_{i,t}(s)}\min_{\mathbf{w}\in\mathcal{W}(u)}\sum_{i=1}^{N}\sum_{c=1}^{C}\left(\langle \mathbf{p}_{i,c},\mathbf{w}\rangle-I_{c}(y_{i})\right)^{2}+\lambda\|\mathbf{w}\|^{2}$$

A new way:

$$\max_{\mathbf{P}(i,t)\in\mathcal{P}_{i,t}(s)}\min_{\mathbf{w}\in\mathcal{W}(u)}\sum_{i=1}^{N}\left\langle \mathbf{w},1-\sum_{c=1}^{C}I_{c}(y_{i})p_{c}(i,t)\right\rangle +\lambda\left\|\mathbf{w}\right\|^{2}$$

We consider only the class probability corresponding to class y_i of the *i*-th training example and find how it is far from 1

A simplified quadratic optimization problem

 The quadratic optimization problem for computing optimal weights

$$\min_{\mathbf{w}\in\mathcal{W}(u)}\left(\lambda \|\mathbf{w}\|^2 - \sum_{t=1}^T w_t \sum_{i=1}^N p_{y_i}^*(i, t)\right)$$

p^{*}_{y_i}(*i*, *t*) are smallest values of probabilities from *extreme* points of *P*_{i,t}(s) (from an imprecise statistical model)

Survival analysis (problem statement)

- It is solved by the Random Survival Forest (RSF)
- Given N training examples $S = \{(\mathbf{x}_1, \delta_1, D_1), ..., (\mathbf{x}_n, \delta_n, D_n)\}, \mathbf{x}_i \in \mathbb{R}^m, y_i \in \{1, ..., C\}$
- D_i indicates time to event of the patient
- If the event of interest is observed, $\delta_i = 1$, (an uncensored observation); if the event is not observed, $\delta_i = 0$ (a censored observation)
- A specific regression problem, where we compute the cumulative hazard estimate $H_k(t)$ for every leaf node k by means of the Nelson-Aalen estimator

Interval-valued hazard estimate

- How to take into account imprecision of the cumulative hazard estimate *H_k(t)*?
- The Nelson-Aalen estimator has a standard 100(1 α)% confidence interval for H_k(t):

$$H_k(t) \pm z_{1-\alpha/2} \cdot \sigma_k(t)$$

where $z_{1-\alpha/2}$ is the $1-\alpha/2$ fractile of the standard normal distribution, $\sigma(t)$ is the variance of the Nelson-Aalen estimator

• We get intervals $\mathcal{B}_k = [\underline{H}_k(t), \overline{H}_k(t)]$

Measure of the model quality

- Now we have a new measure of the model quality
- The C-index estimates how good the model is at ranking survival times
- It estimates the probability that, in a randomly selected pair of patients, the patient that fails first had a worst predicted outcome

$$C = rac{1}{M} \sum_{i:\delta_i=1} \sum_{j:t_i < t_j} \mathbf{1} \left[S(t_i^* | \mathbf{x}_i) > S(t_j^* | \mathbf{x}_j)
ight] o \max$$

Optimization problem with a modified C-index

• Optimization problem with the standard C-index

$$\min_{H_q(t|\mathbf{x})\in\mathcal{B}_q}\max_{\mathbf{w}\in\mathcal{W}(u)}\sum_{(i,j)\in J}\mathbf{1}\left[\sum_{q=1}^T w_q\left(H_q(t_j^*|\mathbf{x}_j) - H_q(t_i^*|\mathbf{x}_i)\right) \ge 0\right]$$

• A modified C-index:

$$C_{\mathsf{new}} = rac{1}{M} \sum_{(i,j) \in J} \left(H_q(t_j^* | \mathbf{x}_j) - H_q(t_i^* | \mathbf{x}_i) \right)$$

• Optimization problem with the modified C-index

$$\max_{H_q(t|\mathbf{x})\in\mathcal{B}_q}\min_{\mathbf{w}\in\mathcal{W}(u)}\sum_{q=1}^T w_q \sum_{(i,j)\in J} \left(H_q(t_i^*|\mathbf{x}_i) - H_q(t_j^*|\mathbf{x}_j)\right)$$

• Finally:

$$\min_{\mathbf{w}\in\mathcal{W}(u)} \left(\sum_{q=1}^{T} w_q B_q^* + \lambda \|\mathbf{w}\|^2 \right)$$

Some numerical experiments



▲□▶ ▲圖▶ ▲匡▶ ▲匡▶ ― 臣 … のへで

◆□▶ ◆□▶ ◆臣▶ ◆臣▶ 臣 のへぐ



Thank you for your attention ?