Local tree methods for classification

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Bayesian statistics in the big data area
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Introduction

Complex statistical models ⇒ **Intractable likelihood**

1. $f(y|\theta) = \int f(y, u|\theta) \mu(du)$ intractable
   - population genetics models, coalescent process
   - EM algorithms, Gibbs sampling, pseudo-marginal MCMC methods, variational approximations

2. $f(y|\theta) = g(y, \theta)/Z(\theta)$ and $Z(\theta)$ intractable
   - Markov random field
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Simulate pseudo-datasets using the Bayesian generative models and compare them to the observed dataset.

Since the Likelihood-free rejection sampler for parameter inference:
- Tavare et al. (1997) Genetics
- Pritchard et al. (1999) Molecular Biology and Evolution

numerous developments:
- regression adjustments,
- more efficient algorithms,
- model choice,
- selection of the summary statistics...
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Most popular and efficient ABC strategy: use of Machine Learning tools on the training set produced with the Bayesian generative model (the reference table)

Fast e-free Inference of Simulation Models with Bayesian Conditional Density Estimation
Papamakarios and Murray (2016) NIPS

Approximate the whole posterior distribution by using Mixture Density Networks (Bishop, 1994) - Gaussian mixture models with parameters calibrated thanks to neural networks

The number of mixture components and the number of hidden layers of the networks require calibration
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Unsupervised pretraining using autoencoders very interesting, but requires a lot of calibration.
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Pudlo, Marin et al. (2016) Bioinformatics

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No tuning parameter, very good properties for sparse problems and heterogeneous predictors (the summary statistics)

RF have theoretical guarantees for sparse problems

Biau (2012) JMLR

Sub-optimal to construct RF able to estimate everywhere in the space of predictor variables

We are only interested in one point, the observed dataset $y^*$

⇒ local approaches
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Here, we focus on model choice problems

We observe $y^*$ and consider $K$ statistical models $\mathcal{M}_1, \ldots, \mathcal{M}_K$ in competition

Prior distributions $\pi(\mathcal{M} = \mathcal{M}_k)$ and $\pi_k(\theta_k)$ on the parameters of model $\mathcal{M}_k$
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**Prior distributions** $\pi(\mathcal{M} = \mathcal{M}_k)$ and $\pi_k(\theta_k)$ on the parameters of model $\mathcal{M}_k$
1 Classification trees and Random Forests

2 ABC model choice via Random Forests

3 Local splitting rules

4 Local weighting of the individuals

5 Local weighting of the predictors

6 Numerical results and discussion
1. **Binary trees**

2. Each internal node splits the training set into two daughter nodes depending on a condition $x^{(j)} \leq s$

3. Predictor $j$ and split value $s$ chosen to maximise an information gain

4. Each terminal node (leaf) predicts a model, the prediction is the majority vote in the leaf where it ends once passed through the tree
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Information gain

\[ \sum_{k=1}^{K} p_k (1-p_k) - \left\{ \frac{N_L}{N_{\text{root}}} \sum_{k=1}^{K} p_{k,L} (1-p_{k,L}) + \frac{N_R}{N_{\text{root}}} \sum_{k=1}^{K} p_{k,R} (1-p_{k,R}) \right\} \]

\( p_k \) corresponds to the proportion of points in the root node associated to the model \( k \)

\( p_{k,L} \) the proportion for the left daughter node

\( p_{k,R} \) the proportion for the right daughter node

Maximize information gain using the Gini impurity \( \sum_{k=1}^{K} p_k (1-p_k) \)

or the Entropy \( -\sum_{k=1}^{K} p_k \log(p_k) \), that’s pretty much the same
Grow a forest of many trees

Grow each tree on an independent bootstrap sample from the training data such that at each node:

1. Select $m$ variables at random out of all predictors
2. Find the best split on the selected $m$ predictors

Vote the trees to get predictions for new data

**Improve on CART with respect to accuracy and stability**
Random Forests

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**Improve on CART with respect to accuracy and stability**
A standard decision tree will split at $x^{(1)} \approx 0.5$
⇒ loosing some interesting datasets for the prediction of $y^*$

We would like to split according to the pertinent predictors for $y^*$
ABC Random Forests

**Input** ABC reference table involving model index and summary statistics, table used as learning set

possibly large collection of summary statistics: from scientific theory input to machine-learning alternatives

For $i = 1, \ldots, N$

a) Generate $m_i$ from the prior $\pi(M = m)$

b) Generate $\theta'_m$ from the prior $\pi_{m_i}(\cdot)$

c) Generate $z_i$ from the model $f_{m_i}(\cdot | \theta'_m)$

d) Calculate $x_i = \eta(z_i)$

**Output** a random forest classifier to infer model indexes $m(\eta(y^*))$
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**Output**  a random forest classifier to infer model indexes $\hat{m}(\eta(y^*))$
Local splitting rules

Change the information gain to the benefit of a more local one

Use $y^*$ to drive the splits and thus the tree construction

Uni-dimensional Kernel approach

Local information gain associated to variable $j$

$$
\sum_{k=1}^{K} \tilde{p}_k (1 - \tilde{p}_k) - \left\{ \frac{\tilde{N}_L}{\tilde{N}_{root}} \sum_{k=1}^{K} (\tilde{p}_{k,L} (1 - \tilde{p}_{k,L}) + \frac{\tilde{N}_R}{\tilde{N}_{root}} \sum_{k=1}^{K} (\tilde{p}_{k,R} (1 - \tilde{p}_{k,R}) \right\}
$$

$$
\tilde{p}_{k,L} = \sum_{i \in LD} K_{h_j} \left( \eta(y^*)^{(j)} - x_i^{(j)} \right) 1_{m_i = k}
$$

$$
\tilde{N}_L = \sum_{i \in \text{ROOT}} K_{h_j} \left( \eta(y^*)^{(j)} - x_i^{(j)} \right) 1_{x_i^{(j)} \leq s}
$$
Local splitting rules

We tried several kernels and bandwidths

That is related to

Lazy Decision Trees
Friedman et al. (1997) Proc. of the 13th National Conference on AAAI
Local weighting of the individuals

**Case-Specific Random Forests**

Xu et al. (2016) Journal of Computational and Graphical Statistics

Produce a first RF with default parameter

Deduce from that RF distances between individuals in the training set and $y^*$

Produce a second RF that uses these weights to modify the bootstrap step

We tried another possibility: identify neighbours using standard distance and then construct a RF on this set of neighbours
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1. Pass $y^*$ through each tree of the RF and count the number of times each has been used in a splitting rule to allocate $y^*$

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Produce a second RF that uses these weights to randomly select the predictors at each node

Weight the predictors: better cuts but increase the correlation between the RF’s trees...
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Numerical results

We tried several examples, for instance, a 20-dimensional Gaussian mixtures with 4 classes and 20 noise predictor variables

Simple enough to compute the Bayes classifier
Numerical results

3,000 instances in the training set, sampled among the four classes with equal probabilities
500 instances as testing set

100 trees in the forests

1. Bayes classifier: 12.6
2. RF: 22.4
3. Local splitting rule: same as RF after tuning
4. Local weighting of the individuals: same as RF after tuning
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Local forest methods do not work as expected

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In a Chinese restaurant, I got a hidden message within a cake. This year, take comfort in your rituals, but be open to new experiences. I was very enthusiastic.

One year latter, back to the real world.... trees methods are extremely difficult to localize.

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