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A Theoretical Analysis of Random Forest Models for Imputation, Prediction and Variable Selection

Dortmund Data Science Center

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Short introduction of myself and my institute

- Burim Ramosaj, graduated at Ulm University and Syracuse University in Mathematics and Management
- PhD-Studies at TU Dortmund University. Thesis title:
  Analyzing Consistency and Statistical Inference in Random Forest Models.
  Supervisor: Prof. Dr. Markus Pauly and Prof. Dr. Jörg Rahnenführer
- Post-doc at the Institute of Mathematical Statistics and Applications in Industry within DFG project PA 2409/3-2.
- From 2021 on: Own project on *Statistical Inference Analysis with Machine Learning* funded from the state of NRW.
- Research focus of our group:
  - Machine Learning (ML) Methods for Inference and Prediction
  - Random Forest and Ensemble Methods
  - Resampling
  - Statistical Inference with Missing Values
  - Survival Analysis and Time Series Analysis

Focus on **Random Forest Models (RF)** for the following purposes:

- Imputing missing values.
- Inference after imputation.
- Uncertainty quantification using Random Forests.
- Consistency and (un-)biasedness for RF based measures and estimators.
- Variable selection with Random Forest based importance measures:
    - Absolute Number of Selection Frequency.
    - Gini Importance.
    - Permutation Importance.
- Combination with Neural Networks (structural relations).

1. Multiple imputation and Random Forest

We focus on imputation procedures, specifically, **multiple imputation (MI)**. It has the following advantages:

- Easy to implement.
- Standard statistical analysis can be applied.
- Theoretical guarantees for its *correct* usage exists (Rubin, 2004).
- Reflects uncertainty of the data generating process.

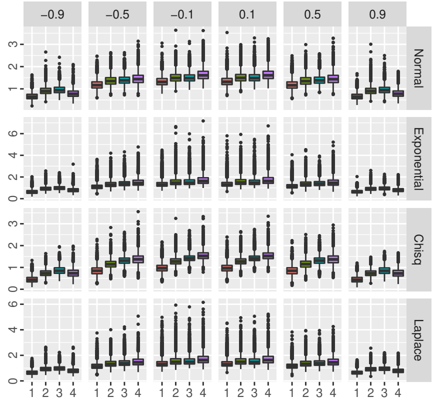
Combination with research and application trend of involving ML-based methods, like the RF:

- No statistical modeling required.
- Treating simultaneously categorical and continuous variables.
- Low tuning efforts with comparably high predictive accuracy.

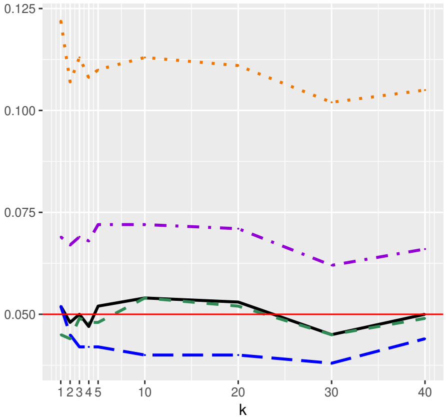
1. Multiple imputation and Random Forest

- Highly cited paper of Stekhoven and Bühlmann (2012) when using `missForest` for imputation (1,390 citations as of today).

We measured imputation accuracy for various techniques (Ramosaj et al., 2020):



- Normalized Root Mean Squared Error (NRMSE) for:
  (1) RFMI, (2) RFMICE, (3) PMM and (4) NORM
- `missForest` performs *best* under the MI framework (RFMI).
- Multiple Imputation Using Chained Equations under the Bayesian regression model with Gaussian assumption (NORM) performs worse.



Measuring **type-I error in paired data**

- T_{ML} (——), RF MI ($\cdots$), RF MICE ($- \cdot -$), PMM ($- -$), NORM ($- - -$) for χ^2 distribution under $\rho = 0.1$ and Σ_1 for varying k values multiplied to $(30, 10, 10)$, i.e. $(n_1, n_2, n_3) = k \cdot (30, 10, 10)$.
- RFMI (`missForest`) highly inflates type-I error.
- Reason: No multiple imputation; incorrect treatment of uncertainty.
- This is even provable (Ramosaj, 2020).

Future research work on imputation

- Influence of the often-used NRMSE (normalized root mean squared error) and PFC (proportion of false classification) measure on the prediction accuracy such as mis-classification and mean-squared error.
- Coverage of prediction intervals after imputation with ML-based imputation techniques.
- General issue of constructing correct and valid prediction intervals.

RF models are also used for selecting **informative** variables.

- Absolute Number of Selection Frequency
- Mean Decrease in Impurity
- Permutation Importance

Simulation-based evidence that RF variable selection is:

- biased (Strobl et al., 2007)

exists. No **theoretical guarantees** so far!

We could show the following results (Ramosaj and Pauly, 2019):

- The permutation importance measure $I_{n,M}^{OOB}(j)$ for regression learning problems is asymptotically **unbiased**, i.e. there is a constant $C > 0$ such that

$$\lim_{n\to\infty} \lim_{M\to\infty} \mathbb{E}[I_{n,M}(j)] = C \cdot \mathbb{1}\{j \in \mathcal{S}\} \tag{1}$$

  and $\mathcal{S}$ is the **informative set**.
- Under slightly stronger assumption, we can also show that

$$I_{n,M}^{OOB}(j) \xrightarrow{\mathbb{P}} C \cdot \mathbb{1}\{j \in \mathcal{S}\}, \text{ as } (n, M) \overset{seq}{\to} \infty. \tag{2}$$

Future research work on variable selection

We aim to detect influential variables through formal testing of:

$$H_0 : I_{n,M}^{OOB}(j) = 0 \quad vs. \quad I_{n,M}^{OOB}(j) \neq 0$$

The following approaches might be considered:

- Parametric approach, i.e. finding an appropriate limit distribution.
- Non-parametric approach by using permutation tests.

We received seperate funding from the state of NRW for this specific research question.

Current collaborations

Thanks to my **collaboration partners**:

Prof. Dr. Markus Pauly
Faculty of Statistics, TUD

Prof. Dr. Jörg Rahnenführer
Faculty of Statistics, TUD

Prof. Dr. Jian-Jia Chen
Faculty of Informatics, TUD

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Ecole Polytechnique

Prof. Dr. Gérard Biau
Sorbonne Center for Artificial Intelligence, Paris

Prof. Dr. Lucas Mentch
Department of Statistics, Pittsburgh University

Thank you for your attention!

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Main issue in statistical inference after imputation:

Correct Uncertainty Quantification

- Use **multiple imputation logic** as given in Rubin (2004): Interested in testing

$$H_0 : \boldsymbol{Q} = \boldsymbol{Q}_0 \quad vs. \quad H_0 : \boldsymbol{Q} \neq \boldsymbol{Q}_0$$

- Generate $m \in \mathbb{N}$ data sets $\mathcal{D}_n^{(1)}, \ldots, \mathcal{D}_n^{(m)}$ from the intial data set.
- Calculate for every data the estimator $\boldsymbol{Q}_{n,t}$ as in standard complete procedures and estimate its variance $\boldsymbol{U}_{n,t}$ similarly.
- Aggregation of the estimator: $\bar{\boldsymbol{Q}}_{n,m} = \frac{1}{m} \sum_{t=1}^{m} \boldsymbol{Q}_{n,t}$ und $\bar{\boldsymbol{U}}_{n,m} = \frac{1}{m} \sum_{t=1}^{m} \boldsymbol{U}_{n,t}$.
- Estimate variance of $\bar{\boldsymbol{Q}}_{n,m}$ through $\bar{\boldsymbol{U}}_{n,m} + (1 + 1/m)\, \boldsymbol{B}_{n,m}$,
  $\boldsymbol{B}_{n,m} = \frac{1}{m-1} \sum_{t=1}^{m} (\boldsymbol{Q}_{n,t} - \bar{\boldsymbol{Q}}_{n,m})(\boldsymbol{Q}_{n,t} - \bar{\boldsymbol{Q}}_{n,m})^\top$.

Appendix: Variable Selection

Random Forest models are also used in variable selection. Different measures do exists:

- Absolute Number of Selection Frequency

$$ABS_{n,M}(j) = \frac{1}{M}\sum_{t=1}^{M}\sum_{k=1}^{t_n-1} \mathbb{1}\{\text{variable } j \text{ selected in tree } t \text{ at node } t_n\}$$

- Mean Decrease in Impurity:

$$MDI_{n,M}(j) = \frac{1}{M}\sum_{t=1}^{M}\sum_{k,s} \frac{|N_n(A_{n,s}^{(k)}(\Theta_t))|}{n} \cdot L_{n,s}^{(k)}(j, z_j) \cdot \mathbb{1}\left\{L_{n,s}^{(k)}[j, z_j] \geq L_{n,s}^{(k)}[\ell, z_\ell], \forall \ell \neq j, z_j, z_\ell\right\}$$

- Permutation Importance:

$$I_{n,M}^{OOB}(j) = \frac{1}{\gamma_n M}\sum_{t=1}^{M}\sum_{i\in\mathcal{D}_n^{(-t)}} \left\{\psi\left(Y_i, m_{n,M}^{OOB}(\mathrm{X}_i^{\pi_{j,t}}; \Theta_t)\right) - \psi\left(Y_i, m_{n,M}^{OOB}(\mathrm{X}_i; \Theta_t)\right)\right\},$$

ψ is some loss function, depending on the context.