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Statistical learning for radioactive waste characterization



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Radiological characterization is needed to dispose of the radioactive waste produced in high energy particle accelerators. We applied statistical learning methods to predict the activity of Difficult-to-Measure radionuclides – which are low-energy X, α- and β-emitters –, to establish criteria for sorting radioactive waste and to quantify prediction errors.

Introduction

DTM Difficult-to-Measure nuclides cannot be easily quantified by non-destructive assay means. Their activity a_{DTM} is often correlated to the concentration of γ -emitters.

CF If a_{DTM} is correlated with the activity a_{KN} of a major γ -emitter - called **Key Nuclide KN** - we can estimate a_{DTM} using a **Correlation Factor CF**:

$$a_{DTM} = CF \times a_{KN}$$

We conducted an extensive numerical experiment to predict the behaviour of CFs.

Simulations

We generated $\sim 2.4 \times 10^6$ CERN activation scenarios. For each scenario:

- We extrapolated the **Radionuclide Inventory** \Rightarrow List of produced nuclides
- We identified the **Key Nuclide**
- We calculated the **Correlation Factor** for each pair DTM/KN

Statistical learning methods

- We used **Decision Trees** and **Multiple Linear Regression** to estimate average CFs and to find possible sorting criteria
- We used **Bagging**, **Random Forests** and **k-fold Cross Validation** to minimize variances and to quantify **Prediction Errors**

ISO Standard 16966. *Theoretical activation calculation method to evaluate the radioactivity of activated waste generated at nuclear reactors* (2013).

Input Space

The features X considered for the statistical models are:

- **Beam Energy** \Rightarrow 6 levels from 160 MeV (Linac 4) up to 7 TeV (LHC)
- **Location Inside Tunnel** \Rightarrow 7 levels
- **Irradiation Time** \Rightarrow Spaced grid from 0.25 up to 30 years
- **Decay Time** \Rightarrow Spaced grid from 1 up to 40 years

Multiple Linear Regression

- We studied the effects of the predictors X_i on CF using linear models:

$$CF = \beta_0 + \sum_{i=1}^p \beta_i X_i + \epsilon$$

- We used **Best Subset Selection**. Features are chosen using \Rightarrow Mallows's C_p coefficient, Bayesian Inference Criteria, Adjusted R^2 or Akaike Information Criterion
- We found that:

- \Rightarrow **Decay and Irradiation Times** are the **strongest predictors**
- \Rightarrow **5 levels of Beam Energy** - with the exception of 160 MeV - **can be grouped**
- \Rightarrow The feature **Position** inside the tunnel **plays a minor role** when predicting CFs

Prediction Error using k-fold Cross-Validation

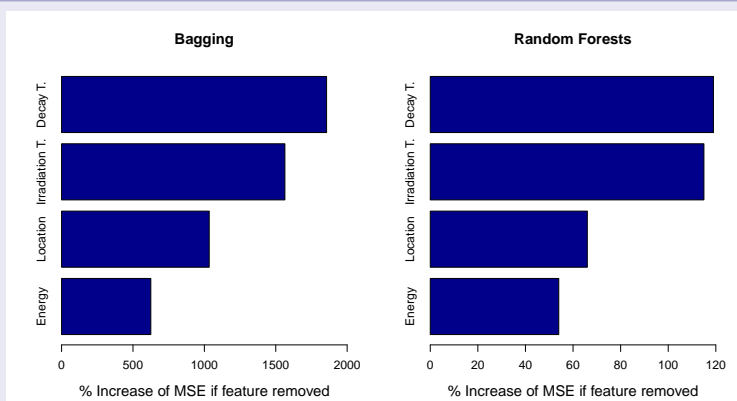
- We used **k-fold Cross-Validation** $CV_{(k)}$ to estimate **Prediction Error**
- Scenarios are randomly divided into k groups
- The model is fit on $k-1$ folds and MSE is calculated in the held-out fold
- The **k-fold CV estimate** is computed by averaging the calculated MSE:

$$CV_{(k)} = \frac{1}{k} \sum_{i=1}^k MSE_i$$

Example: The prediction error $CV_{(10)}$ for $CF(^3H/^{22}Na)$ in Aluminium 6060, when all predictors are included, is 0.26 \Rightarrow The average CF is affected by an error $e^{0.26} = 1.3$

C.M. Bishop, *Pattern recognition and machine learning*, Springer (2006).

Figure 2: Variable importance for $CF(^3H/^{22}Na)$ in Aluminium 6060



The importance of a variable is estimated as the **Percentage Increase of MSE** if the variable is removed from the model

Regression Trees

- We used **Regression Trees** to identify groups of CFs using **Binary Splitting**
- The feature used to split minimizes the **Residual Standard Errors**
- **Mean CFs** are calculated at each node of the tree (red boxes in Figure 1)

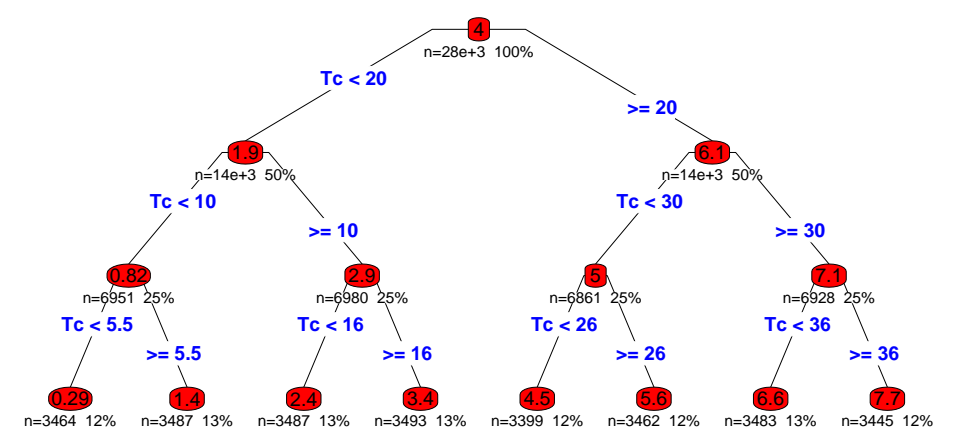
Log-transformation, Training and Test data sets, Prediction Error

- The distribution of calculated CFs is **log-normal** \Rightarrow The logarithm of the data is calculated to normalize the observations
- The n data is split into **training data set** ($m = n/2$) and **test data set** ($m = n/2$) to build the tree and estimate the error on a new prediction
- The **Prediction Error** is the square root of the **Mean Squared Error of Residuals**:

$$MSE = \frac{1}{m} \sum_{i=1}^m (y_i - \hat{f}(x_i))^2$$

Example: The prediction error of the regression tree in Figure 1 is 0.62 \Rightarrow The average CF is affected by an error $e^{0.62} = 1.86$.

Figure 1: Regression Tree of $CF(^3H/^{22}Na)$ in Aluminium 6060



- $T_c \Rightarrow$ Decay Time
- $n \Rightarrow$ Number of scenarios in training set
- **4** \Rightarrow Logarithm of the Correlation Factor

Variance Reduction using Bagging and Random Forests

Decision trees are often affected by high-variance \Rightarrow Different training data sets generate very different outputs.

- We applied 2 known variance reduction techniques to reduce output variability
- We calculated the MSEs and we identified the method that minimizes the error

Bagging

- This method aggregates decision trees obtained by **Bootstrapping** observations from the training data set
- The prediction error is calculated on the left-out bootstrapped data

Example: The prediction error of the bagged tree of $CF(^3H/^{22}Na)$ is 0.0062 \Rightarrow Bagging reduces the variance of 2 orders of magnitude!

Random Forests

- This technique is similar to bagging but it forces each split to consider only a subset of predictors \Rightarrow The trees are decorrelated

Example: The prediction error obtained applying random forests for $CF(^3H/^{22}Na)$ is 0.61 \Rightarrow No major improvement from the regression tree.

T. Hastie, R. Tibshirani and J. Friedman. *The elements of statistical learning. Data Mining, Inference, and Prediction*, 2nd Ed., Springer (2009).

Conclusions

To characterize radioactive waste produced in high-energy particle accelerators we must estimate the list of radionuclides produced (α -, β - and γ -emitters) and their activities.

- We estimated the **activity of Difficult-to-Measure nuclides** using the **Correlation Method**
- We used **Regression Trees** and **Linear Models** to predict **Correlation Factors**
- We applied **Bagging**, **Random Forests** and **k-fold Cross-Validation** to estimate **Prediction Errors**
- We identified **splitting variables at the nodes** of the regression trees as potential **sorting criteria** for radioactive waste