Variable Importance Measures for Functional Gradient Descent Boosting Algorithm

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Zeyu Ding, Faculty of Statistics

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Introduction

Challenges in statistics as variables increase

High-dimensional Data

- Number of variables $p$ is much higher than the number of samples $n$
Introduction

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Overly complex models
- High performance, low interpretability
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Challenges in statistics as variables increase
High-dimensional Data
  - Number of variables $p$ is much higher than the number of samples $n$

Overly complex models
  - High performance, low interpretability

Overfitting
  - Model performs well in the training phase and the prediction accuracy is however weak
Introduction

Solutions to these problems
Model Selection

- AIC/BIC based model selection methods
Introduction

Solutions to these problems

Model Selection
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Sparse Regression
- Lasso and Ridge based regression methods
Introduction

Solutions to these problems

Model Selection

- AIC/BIC based model selection methods

Sparse Regression

- Lasso and Ridge based regression methods

Variable Importance Measures

- Usually used in ensemble algorithm, i.e., Random Forest, Gradient Boosting
Methodology

Functional Gradient Descent Boosting Algorithm

Statistical Boosting

- Gradient boosting algorithm can be viewed as a statistical model of the generalized additive model class.

\[ f(x) = \beta_0 + f_1(x_1) + f_2(x_2) + \cdots + f_p(x_p) \]
Methodology

Functional Gradient Descent Boosting Algorithm

Statistical Boosting

- Gradient boosting algorithm can be viewed as a statistical model of the generalized additive model class.

Component-wise gradient boosting

- Only the best performed base-learner is chosen into the model in every iteration.

\[ f(x) = \beta_0 + f_1(x_1) + f_2(x_2) + \cdots + f_p(x_p) \]
Methodology

Functional Gradient Descent Boosting Algorithm

Statistical Boosting

- Gradient boosting algorithm can be viewed as a statistical model of the generalized additive model class.

Component-wise gradient boosting

- Only the best performed base-learner is chosen into the model in every iteration.

Regressed iteratively

- The model complexity is controlled by the number of iteration.

\[ f(x) = \beta_0 + f_1(x_1) + f_2(x_2) + \cdots + f_p(x_p) \]
Methodology

Component-Wise Gradient Boosting Algorithm
1. Set the initial iteration $m=0$. Given the initialized value of $\hat{f}[0](\cdots)$, common choices are

$$\hat{f}[0] \equiv \arg \min_c \frac{1}{n} \sum_{i=1}^{n} \rho(Y_i, c)$$

or $\hat{f}[0] \equiv 0$.

2. For $m = 1$ to $m_{\text{stop}}$
   (a). Obtain the negative gradient vector at the previous iteration $m-1$

$$g^{[m]} = g_i^{[m]} = \left( \frac{\partial \rho(y_i, f(x_i))}{\partial f(x_i)} \right)_{f(x_i) = f_{m-1}(x_i)} (i=1, \ldots, n)$$

(b). Fit the negative gradient vector $g^{[m]}$ to the input variables $x$ by the base-learner procedure.

$$(x_1, g^{[m]}), (x_2, g^{[m]}), \ldots, (x_p, g^{[m]}) \xrightarrow{\text{procedure}} \hat{h}^m_i(x_i)_{i=1, \ldots, p}$$
Methodology

Component-Wise Gradient Boosting Algorithm

(c). Select the component $j^*$ that best fits the negative gradient vector $g_m$

$$j^* = \arg \min_{1 \leq j \leq p} \sum_{i=1}^{n} (g_i^m - \hat{h}_j^m(x_j))^2$$

(d). The model $\hat{f}^m(\cdot)$ is updated by

$$\hat{f}^m(\cdot) = \hat{f}^{m-1}(\cdot) + \theta \cdot \hat{h}_j^m(x_{j^*})$$

where $\theta$ denotes a step length.

3. After $m_{stop}$ iterations, the model is obtained by

$$\hat{f}(\cdot) = \hat{f}^m(\cdot)$$
Methodology

Variable Selection Criterion
Selection Frequency

- Currently implemented in the algorithm
Methodology

Variable Selection Criterion

Empirical Risk Reduction

- The empirical risk reduction from each base learner in every iteration is calculated

\[ V_{\text{risk}}^{[j]}(\hat{h}_j(\cdot)) = \sum_{m:j^*_m} (\rho(y, \hat{f}[m]) - \rho(y, \hat{f}[m-1])) \]

\( l^2 \)-norm Contribution

- The \( l^2 \)-norm of every base-learner is used as a measure of the variable importance

\[ \|\hat{h}_j(\cdot)\| = \sqrt{\sum_{i=1}^{n} (\hat{h}_j[m_{\text{stop}}](x_{ij}))^2} \]

\[ V_{\text{norm}}^{[j]}(\hat{h}_j(\cdot)) = \frac{\|\hat{h}_j(\cdot)\|}{\sum_{j=1}^{p} \|\hat{h}_j(\cdot)\|} \]
Simulation Data

Linear Model
- Simple Linear Model as base learners

Non-linear Model
- B-spline as base learners

Table 3: Sample size $n$ and number of iterations $m_{stop}$

<table>
<thead>
<tr>
<th>Sample size $n$</th>
<th>number of iterations $m_{stop}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n = 50$</td>
<td>$m_{stop} = 40$</td>
</tr>
<tr>
<td></td>
<td>$m_{stop} = m_{[cvrisk]}$</td>
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<td>$m_{stop} = 500$</td>
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<td>$n = 200$</td>
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</tr>
<tr>
<td></td>
<td>$m_{stop} = 500$</td>
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</tbody>
</table>
Simulation Data
High-Dimensional Data

Table 5: Simulation design for high-dimensional scenario

<table>
<thead>
<tr>
<th>Sample size $n$</th>
<th>number of influential variables $k$</th>
<th>number of non-influential variables $j$</th>
<th>number of variables $p$</th>
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<td>$n = 50$</td>
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Main Result

Linear Model

(a) change in variable coefficients
(b) change in selection frequency
(c) change in risk reduction
(d) change in norm contribution
Main Result

High-dimensional Data

Figure 31: Number of false positive variables in high-dimensional scenario
Conclusion

Overfitting

- The variable importance measures based on empirical risk reduction and norm contribution in the FGDB algorithm are stable in resisting overfitting problem.
Conclusion

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High-Dimensional Data

- In high-dimensional data scenario, VI risk and VI norm also have a good ability to distinguish and rank variables by their importance.
Conclusion

Overfitting

- The variable importance measures based on empirical risk reduction and norm contribution in the FGDB algorithm are stable in resisting overfitting problem.

High-Dimensional Data

- In high-dimensional data scenario, VI risk and VI norm also have a good ability to distinguish and rank variables by their importance.

Multicollinearity

- They are also stable when existing multicollinear variables.
Outlook

More Complex Data

- In future research, more complex data scenarios need to be considered.

More Real-World Applications

- More real-world data needs to be validated, especially in the field of biometrics and bioinformatics when the dimensionality of the data is very high.
Outlook

More Complex Data

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More Real-World Applications

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Thanks for your attention!
Reference


Reference


Appendix
Boston House Price Data

<table>
<thead>
<tr>
<th>Variable abbreviation</th>
<th>Variable explanation</th>
</tr>
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<tbody>
<tr>
<td>crim</td>
<td>per capita crime rate by town</td>
</tr>
<tr>
<td>zn</td>
<td>proportion of residential land zoned for lots over 25,000 sq.ft</td>
</tr>
<tr>
<td>indus</td>
<td>proportion of non-retail business acres per town</td>
</tr>
<tr>
<td>chas</td>
<td>Charles River dummy variable (= 1 if tract bounds river; 0 otherwise)</td>
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<tr>
<td>nox</td>
<td>nitrogen oxides concentration (parts per 10 million)</td>
</tr>
<tr>
<td>rm</td>
<td>average number of rooms per dwelling</td>
</tr>
<tr>
<td>age</td>
<td>proportion of owner-occupied units built prior to 1940</td>
</tr>
<tr>
<td>dis</td>
<td>weighted mean of distances to five Boston employment centres</td>
</tr>
<tr>
<td>rad</td>
<td>index of accessibility to radial highways</td>
</tr>
<tr>
<td>tax</td>
<td>full-value property-tax rate per $10,000</td>
</tr>
<tr>
<td>ptratio</td>
<td>pupil-teacher ratio by town</td>
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<tr>
<td>black</td>
<td>$1000(Bk - 0.63)^2$ where $Bk$ is the proportion of blacks by town</td>
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<tr>
<td>lstat</td>
<td>lower status of the population (percent)</td>
</tr>
<tr>
<td>medv</td>
<td>median value of owner-occupied homes in $1000s</td>
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</tbody>
</table>
Appendix

Boston House Price Data

(a) Variable importance by $V_{\text{risk}}$

(b) Variable importance by $V_{\text{norm}}$

(c) Variable importance by Selection frequency

Figure 36: Relative importance result of FGDB algorithm
Appendix

Boston House Price Data

<table>
<thead>
<tr>
<th>Variable</th>
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<th>randomForest</th>
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