Tree-based Machine Learning in Survey Research

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UN Stats Division Brown Bag 11/20/2019

Outline

Introduction

- Machine learning (ML) methods provide a vast set of tools for exploring and analyzing diverse data
- Comprise flexible/ non-parametric methods that adapt to complex data structures
- Focus on out-of-sample prediction performance
  - Learn $f(x)$ with training set $\rightarrow$ predict on test set

- ML increasingly used by survey researchers in various contexts (Buskirk et al. 2018, Kern et al. 2019)
- A promising *supplement* in the survey methods toolkit

$\rightarrow$ This talk focuses on **tree-based methods** as an important subgroup of ML methods

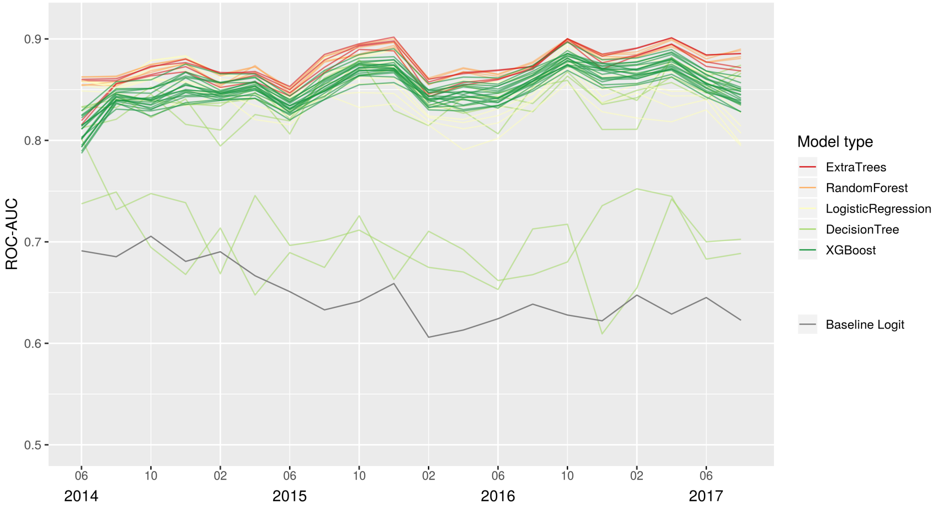
ML and Survey Research

Some examples

- Create sampling frame based on satellite images (Eckman and Qiu 2019)
- Estimate response propensities for weighting (Buskirk and Kolenikov 2015)
- Predict matches in record linkage (Schild et al. 2017)
- Create synthetic data (Drechsler and Reiter 2011)
- Predict nonreponse in panel surveys (Kern et al. 2019)
- Estimate propensity scores (McCaffrey et al. 2004)

ML and Survey Research

Figure: Predicting panel nonresponse with different model types[1]



[1] https://arxiv.org/abs/1909.13361

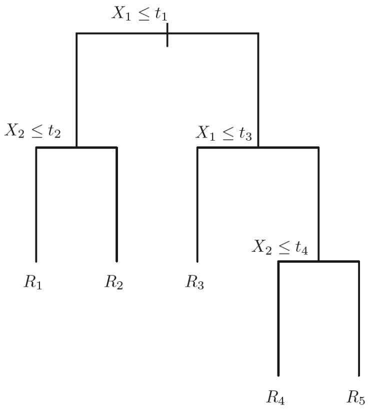
Tree-based (Ensemble) Methods

Classification and Regression Trees (CART)

Decision Trees

- Approach for partitioning the predictor space into smaller subregions
- Results in a "top-down" tree structure
- Important building block (base learner) for ensemble methods
- Many different tree building algorithms exist (Loh 2014)
  - **CART**, CHAID, CTREE...

Figure: A small tree



Tree growing

Growing a **regression tree**

Define pairs of regions for all $X_1, X_2, ..., X_p$ predictors and cutpoints c

$$\tau_L(j, c) = \{X | X_j < c\} \text{ and } \tau_R(j, c) = \{X | X_j \geq c\}$$

Find split s which maximizes the reduction in RSS

$$\Delta RSS(s, \tau) = RSS(\tau) - RSS(\tau_L) - RSS(\tau_R)$$

$$RSS(\tau) = \sum_{i \in \tau} (y_i - \hat{y})^2$$

with $\hat{y}$ being the mean of y in node τ

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Growing a **regression tree**

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Tree growing

Growing a **classification tree**

Find split s which maximizes the reduction in node impurity

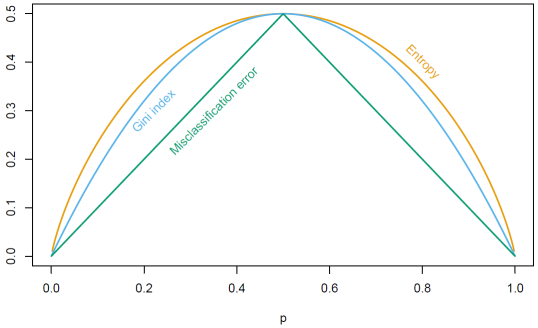
$$\Delta I(s,\tau) = I(\tau) - p(\tau_L)I(\tau_L) - p(\tau_R)I(\tau_R)$$

Gini Impurity

$$I_{Gini}(\tau) = \sum_{k=1}^{K} \hat{p}_k(1-\hat{p}_k)$$

with $\hat{p}_k$ being the proportion of observations from class k in node τ

Figure: Impurity measures (Hastie et al. 2009)



Tree growing

Algorithm 1: Tree growing process

```
Define stopping criteria;
Assign training data to root node;
if stopping criterion is reached then
    end splitting;
else
    find the optimal split point;
    split node into two subnodes at this split point;
    for each node of the current tree do
        continue tree growing process;
    end
end
```

Tree structure

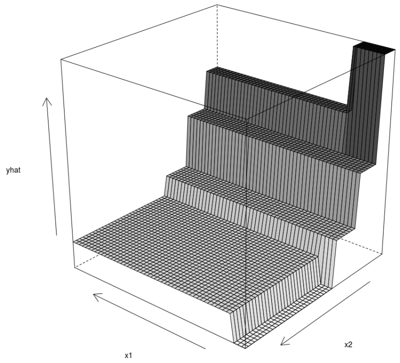
A given tree

$$\mathcal{T} = \sum_{m=1}^{M} \gamma_m \cdot 1_{(i \in \tau_m)}$$

consists of a set of $m = 1, 2, \ldots, M$ nodes which can be used for prediction by...

- Regression
  - ...using the mean of y for training observations in τ_m
- Classification
  - ...going with the majority class in τ_m

Figure: Tree prediction surface



Tree pruning

Stopping rules

- Minimum number of cases in terminal nodes
- Decrease in impurity exceeds some threshold

$\rightarrow$ However, worthless splits can be followed by good splits

Cost complexity pruning

$$R_\alpha(\mathcal{T}) = R(\mathcal{T}) + \alpha|\mathcal{T}|$$

- Find the best subtree by balancing quality $R(\mathcal{T})$ and complexity $|\mathcal{T}|$
- α controls the penalty on the number of terminal nodes
- α can be chosen through CV

Bagging and Random Forest

Bagging Trees

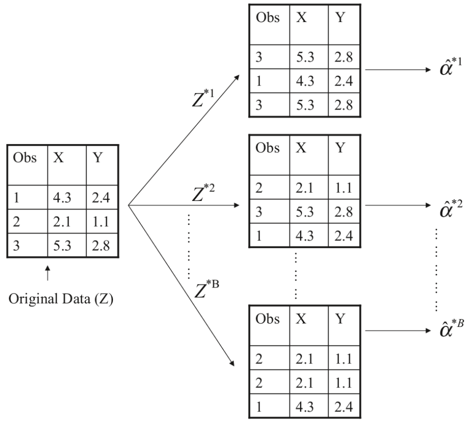
Some limitations of CART

- Lack of smoothness of prediction surface
- High variance/ instability due to hierarchical splitting process

→ **Ensemble methods**

- Address instability via combining multiple prediction models
- Combine diverse models into a more robust ensemble
- e.g. **Bagging**: Bootstrap Aggregating

Figure: Bootstrap process (James et al. 2013)



Bagging Trees

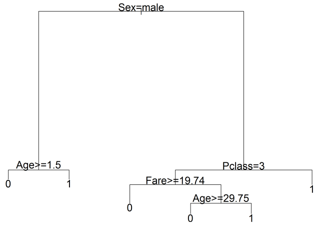
Algorithm 2: Bagging Trees

```
1  Set number of trees $B$;
2  Define stopping criteria;
3  for $b = 1$ to $B$ do
4      draw a bootstrap sample from the training data;
5      assign sampled data to root node;
6      if stopping criterion is reached then
7          end splitting;
8      else
9          find the optimal split point among the predictor space;
10         split node into two subnodes at this split point;
11         for each node of the current tree do
12             continue tree growing process;
13         end
14     end
15 end
```

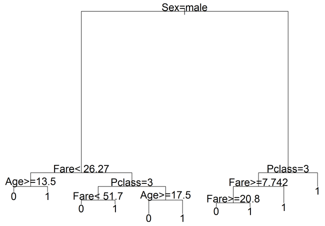
Bagging Trees

Figure: Bagging Trees

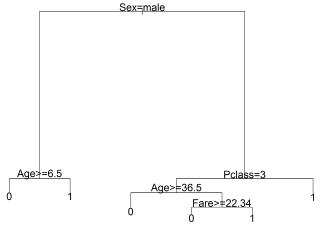
(a) b = 1



(b) b = 2



(c) b = 3



Random Forests

From Bagging to Random Forests

Variance of an average of B i.i.d. random variables

$$\frac{1}{B}\sigma^2$$

$\rightarrow$ Bagging: Averaging over B trees decreases variance

Variance of an average of B i.d. random variables with $\rho > 0$

$$\rho\sigma^2 + \frac{1-\rho}{B}\sigma^2$$

$\rightarrow$ **Random Forests**: Averaging over B trees with m out of p predictors per split decreases variance and decorrelates trees

Random Forests

From Bagging to Random Forests

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Variance of an average of B i.d. random variables with $\rho > 0$

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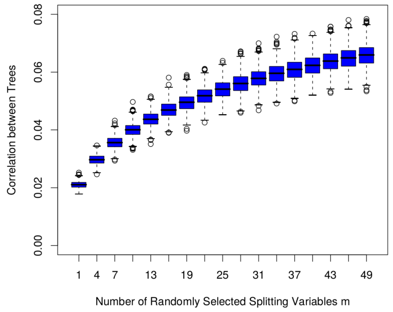
$\rightarrow$ **Random Forests**: Averaging over B trees with m out of p predictors per split decreases variance and decorrelates trees

Random Forests

The Random Forest trick (Breiman 2001)

- Randomization with respect to rows *and* columns
- Weaker predictors have more of a chance
- Results in diverse and *decorrelated* trees

Figure: Correlations between pairs of trees (Hastie et al. 2009)



Growing a Forest

Algorithm 3: Grow a Random Forest

```
Set number of trees $B$;
Set predictor subset size $m$;
Define stopping criteria;
for $b = 1$ to $B$ do
    draw a bootstrap sample from the training data;
    assign sampled data to root node;
    if stopping criterion is reached then
        end splitting;
    else
        draw a random sample $m$ from the $p$ predictors;
        find the optimal split point among $m$;
        split node into two subnodes at this split point;
        for each node of the current tree do
            continue tree growing process;
        end
    end
end
```

Growing a Forest

A Random Forest

$$\{\mathcal{T}_b\}_1^B$$

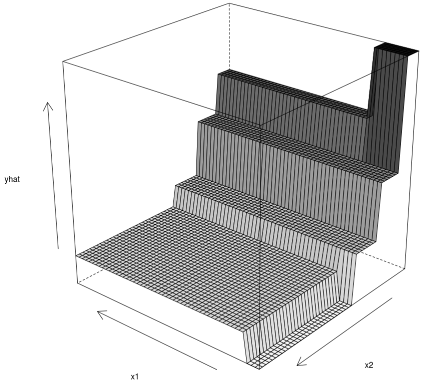
consists of a set of $b = 1, 2, \ldots, B$ trees which can be used for prediction by...

- Regression
  - Averaging predictions over all trees
  - $\hat{f}_{rf}^B(x) = \frac{1}{B}\sum_{b=1}^B \mathcal{T}_b(x)$
- Classification
  - Using most commonly occurring class among all trees
  - $\hat{C}_{rf}^B(x) = \text{majority vote}\{\hat{C}_b(x)\}_1^B$
- Probability estimation
  - Using the proportion of class votes of all trees
  - Averaging predicted probabilities over all trees

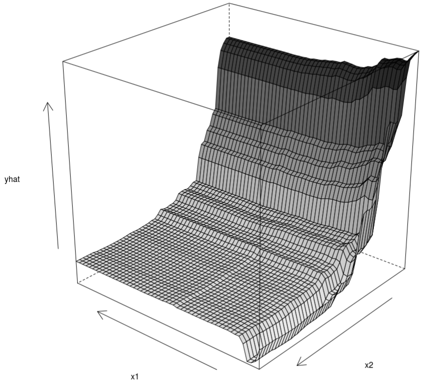
RF vs. CART

Figure: Prediction surface (example)

(a) CART



(b) Random Forest



Tuning RF

Tuning Random Forests

- Predictor subset size m out of p (`mtry`)
  - Most important tuning parameter in RF
  - Starting value; $m = \sqrt{p}$ (classification), $m = p/3$ (regression)
  - Can be chosen using OOB errors based on different m
- Number of trees
  - sufficiently high (e.g. 500)
- Node size (number of observations in terminal nodes)
  - sufficiently low (e.g. 5)

Boosting

Boosting

Boosting methods

- Class of ensemble methods which combine **sequential** prediction models
- Adaptive approach with focus on “difficult observations”
- Different flavors exist
  - AdaBoost
  - Gradient Boosting Machines (GBM)
  - XGBoost
  - ...
- Can be applied to different (weak) base learners
  - Boosting trees
  - Model-based boosting
  - ...

AdaBoost

- Algorithm for classification problems ($Y \in \{-1, 1\}$)
- Estimate a sequence of classifiers using reweighted data
- **AdaBoost process**
  1. Fit classifier $G_m(x)$ to weighted data (intitial weights $w_i = \frac{1}{n}$)
  2. Compute the misclassification rate

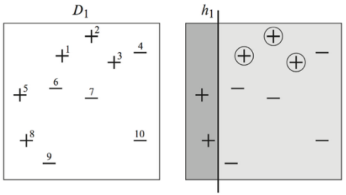
$$\text{err}_m = \frac{\sum_{i=1}^{n} w_i I(y_i \neq G_m(x_i))}{\sum_{i=1}^{n} w_i}$$

  3. Compute the classifier weight $\alpha_m = \log((1 - \text{err}_m)/\text{err}_m)$
  4. Recalculate weights $w_i = w_i \exp(\alpha_m I(y_i \neq G_m(x_i)))$
- Majority vote classification: $G(x) = \text{sign}\left[\sum_{m=1}^{M} \alpha_m G_m(x)\right]$

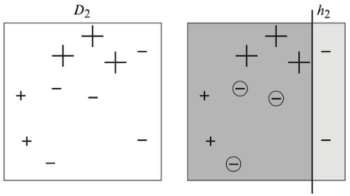
Boosting Stumps

Figure: (Ada)Boosting stumps (example)[2]

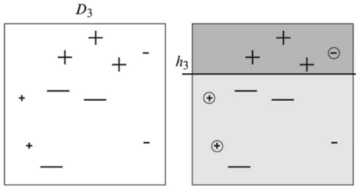
(a) Step 1: $\alpha_1 = 0.42$



(b) Step 2: $\alpha_2 = 0.65$



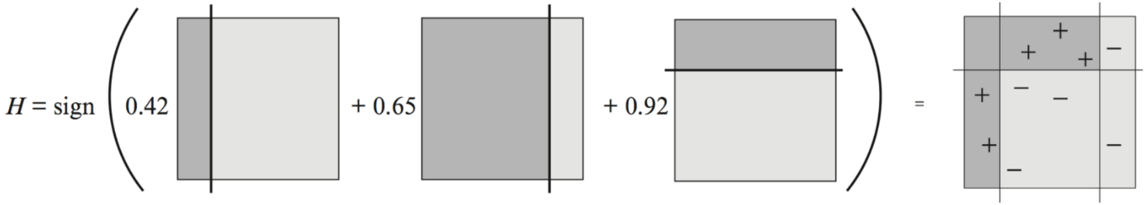
(c) Step 3: $\alpha_3 = 0.92$



[2] Source: Shapire & Freund 2012

Boosting Stumps

Figure: Step 4: Combine models



Gradient Boosting Machines

- General approach to sequential learning
- Applicable with various loss functions
- **Boosting trees**
  1. Initialize model (with a constant $f_0(x)$)
  2. Compute pseudo-residuals based on current model

$$r_{im} = -\left[\frac{\partial L(y_i, f(x_i))}{\partial f(x_i)}\right]_{f=f_{m-1}}$$

  3. Fit a regression tree to the pseudo-residuals
  4. Compute $\gamma_{jm} = \arg\min_\gamma \sum_{x_i \in R_{jm}} L(y_i, f_{m-1}(x_i) + \gamma)$
  5. Update the current model: $f_m(x) = f_{m-1}(x) + \sum_{j=1}^{J_m} \gamma_{jm} I(x \in R_{jm})$
- Output $\hat{f}(x) = f_M(x)$

$\rightarrow$ Analogue to steepest descent

Gradient Boosting Machines

Table: GBM components for different loss functions

Setting	Loss function	r_i	$f_0(x)$
Regression	$\frac{1}{2}(y_i - f(x_i))^2$	$y_i - f(x_i)$	mean(y_i)
Regression	$\lvert y_i - f(x_i) \rvert$	sign$(y_i - f(x_i))$	median(y_i)
Classification	Deviance	$I(y_i = G_k) - p_k(x_i)$	prior p's

Shrinkage, Subsampling, Tuning

Shrinkage

- Additional tweak in Gradient boosting
- Slow down learning rate to avoid overfitting
- Learning rate is controlled by λ
    - $f_m(x) = f_{m-1}(x) + \lambda \sum_{j=1}^{J_m} \gamma_{jm} I(x \in R_{jm})$

Subsampling

- Optional add-on in Gradient boosting
- Use a random sample (w/o replacement) of pseudo-residuals in each step
- Can be introduced to improve performance and speed
    - "Stochastic gradient boosting"

Shrinkage, Subsampling, Tuning

Tuning Gradient Boosting Machines

- Number of trees M
    - Number of "iterations"
    - Overfitting can occur for large M
- Interaction depth D
    - Number of splits for each tree
    - Boosting stumps: $D = 1$
- Shrinkage parameter λ
    - e.g. $\lambda = 0.01$, $\lambda = 0.001$
    - Smaller λ needs larger M
- ...

Boosting for Regression

Algorithm 4: Gradient Boosting for regression

```
1  Set number of trees $M$;
2  Set interaction depth $D$;
3  Set shrinkage parameter $\lambda$;
4  Use $\bar{y}$ as initial prediction;
5  for $m = 1$ to $M$ do
6      compute residuals based on current predictions;
7      assign data to root node, using the residuals as the outcome;
8      while current tree depth $< D$ do
9          tree growing process;
10     end
11     compute the predicted values of the current tree;
12     add the shrinked new predictions to the previous predicted values;
13 end
```

Interpretable ML

Interpretable ML

Interpreting Random Forests, Boosting models

- Inspect each tree of the ensemble
  - Inefficient for 500+ trees
- Variable importance
  - Summary of “effect size”
- Partial dependence plots
  - Graphical representation of “effect structure”
- ...

Variable Importance

Variable importance with CART

$$\mathcal{I}_\ell^2(T) = \sum_{t=1}^{J-1} \hat{\imath}_t^2 I(v(t) = \ell)$$

- Sum of squared improvements $\hat{\imath}^2$ over all internal nodes with predictor X_ℓ
  - Regression: Overall reduction in RSS caused by X_ℓ
  - Classification: Overall reduction of impurity caused by X_ℓ

Importance with Random Forests

$$\mathcal{I}_\ell^2 = \frac{1}{M} \sum_{m=1}^{M} \mathcal{I}_\ell^2(T_m)$$

- Average improvement caused by predictor X_ℓ over all trees

Variable Importance

Permutation feature importance (Fisher et al. 2018)

1. Estimate the original model error $e_{orig}(\hat{f}) = L(Y, \hat{f}(X))$
2. For each feature $j \in 1, \ldots, p$
    1. Generate feature matrix $X_{perm\,j}$ by permuting the values of feature X_j in X
    2. Estimate error $e_{perm} = L(Y, \hat{f}(X_{perm\,j}))$ based on the predictions of the permuted data
    3. Calculate permutation feature importance $FI_j = \frac{e_{perm}(\hat{f})}{e_{orig}(\hat{f})}$ or via $FI_j = e_{perm}(\hat{f}) - e_{orig}(\hat{f})$
3. Output FI for all variables

Partial Dependence Plots

Plotting feature effects in “black box” learning methods

1. Choose a range of values $\{x_{11}, x_{12}, \ldots, x_{1k}\}$ of x_1
2. For each $i \in \{1, 2, \ldots, k\}$
    1. Generate an artificial dataset by fixing x_1 to x_{1i} for all cases
    2. Compute predictions for all cases using the prediction model (e.g. RF)
    3. Average the predictions over all cases
3. Plot the obtained average predictions against x_{1i} for $i = 1, 2, \ldots, k$

ICE and ALE

ICE plots (Goldstein et al. 2014)

- Individual PDPs for all cases w/o final averaging
- One line represents the predictions for one case over the range of x
- Can uncover heterogeneous effects that are driven by interactions
- Centered ICE plots
  - Adjust for different individual baselines

ALE plots (Apley 2016)

- With correlated features, PDPs can (artificially) construct very unlikely combinations
- ALE solution:
  1. Use only cases with (similar) x-values within a given interval
  2. Calculate differences in predictions between upper and lower limit of this interval

More interpretable ML

- Global and local surrogate models
  - `https://arxiv.org/abs/1602.04938`
- Shapley values and SHAP
  - `https://arxiv.org/abs/1705.07874`
- Feature interaction (H-statistic)
  - `https://arxiv.org/abs/0811.1679`
- Partial dependence-based variable importance
  - `https://arxiv.org/pdf/1805.04755.pdf`
- Representative trees from ensembles
  - `https://www.ncbi.nlm.nih.gov/pubmed/22302520`

Summary and Resources

Summary

Tree methods

- Divide-and-conquer strategy that splits the data into subgroups
- No need to specify the functional form in advance (unlike regression)
- Non-linearities and interactions are handled automatically
- Limitations of CART: Instability, competition among correlated predictors, biased variable selection
- Bagging, RF stabilize predictions from high-variance methods
- Boosting sequentially combines multiple models into a powerful ensemble

Software Resources

Resources for R

- Standard package to build CARTs: `rpart`
  - Unified infrastructure for tree representation: `partykit`
- Standard package to grow RFs: `randomForest`
  - Fast implementation of RFs: `ranger`
- Standard package for Gradient Boosting: `gbm`
  - Extreme Gradient Boosting: `xgboost`
- Interpretable Machine Learning in R: `iml`

Books

Hastie, T., Tibshirani, R., Friedman, J. (2009). *The Elements of Statistical Learning: Data Mining, Inference, and Prediction*. New York, NY: Springer.

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Contact

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