Research questions Tree-based methods: application to economics

Pierre Michel







2018-2019 Master in economics (2nd year)

- 1 Introduction
- 2 Tree-based methods
- 3 Advanced tree-based methods
- 4 Applications to Economics: Causal Trees







Tree-based methods: application to economics

-Introduction

1 Introduction
Machine Learning
Machine Learning in economics







Introduction

Machine Learning

What is Machine Learning?

 Machine Learning (ML): field of computer science, statistics and Al







What is Machine Learning?

- Machine Learning (ML): field of computer science, statistics and Al
- Development, analysis and implementation of computational methods







What is Machine Learning?

- Machine Learning (ML): field of computer science, statistics and Al
- Development, analysis and implementation of computational methods
- Allows a machine to evoluates in a given environment through a training process







Applications of Machine Learning?

Use examples:

- Pattern recognition (objects, hand-written characters)
- Clustering of phone-calls
- Medical and clinical decision making
- Web mining, search engines
- Image indexation







The impact of machine learning on economics

"I believe that ML will have a dramatic impact on the field of economics within a short time frame."

— Susan Athey, The Impact of Machine Learning on Economics, 2018.







The impact of machine learning on economics

Applications of ML in many fields of economics:

- Econometrics
- Health economics
- Labour economics
- Housing economics
- Economics of the internet



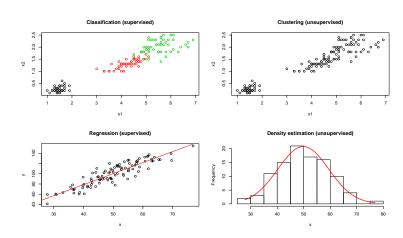




Introduction

└ Machine Learning in economics

Supervised versus Unsupervised learning









Tree-based methods: application to economics

Tree-based methods

2 Tree-based methods Binary trees Regression trees Classification trees







Tree-based methods: application to economics

Tree-based methods

☐Binary trees

Decision trees

Tree-based methods (also called **decision trees**) aim to:







Binary trees

Decision trees

Tree-based methods (also called **decision trees**) aim to:

• partition the feature space into a set of regions.







☐Binary trees

Decision trees

Tree-based methods (also called **decision trees**) aim to:

- partition the feature space into a set of regions.
- fit a simple model in each region.







☐Binary trees

Decision trees

Tree-based methods (also called **decision trees**) aim to:

- partition the feature space into a set of regions.
- fit a simple model in each region.
- useful for regression, classification, clustering.







☐Binary trees

Decision trees

Tree-based methods (also called **decision trees**) aim to:

- partition the feature space into a set of regions.
- **fit** a simple model in each region.
- useful for regression, classification, clustering.

They are **simple** and **powerful**.







Binary trees

Decision trees

Tree-based methods (also called **decision trees**) aim to:

- partition the feature space into a set of regions.
- fit a simple model in each region.
- useful for regression, classification, clustering.

They are **simple** and **powerful**.

Most popular method: Classification and Regression Trees (CART), Breiman, 1984.







Tree-based methods

Regression trees

Building a regression tree

Suppose we have a set of n observations described by p features $X_1, X_2, ..., X_p$ and one **quantitative** response variable Y.







Suppose we have a set of n observations described by p features $X_1, X_2, ..., X_p$ and one **quantitative** response variable Y.

There are two steps for building a tree:







Suppose we have a set of n observations described by p features $X_1, X_2, ..., X_p$ and one **quantitative** response variable Y.

There are two steps for building a tree:

• Divide the feature space in J non-overlapping regions $R_1, R_2, ..., R_J$.







Suppose we have a set of n observations described by p features $X_1, X_2, ..., X_p$ and one **quantitative** response variable Y.

There are two steps for building a tree:

- Divide the feature space in J non-overlapping regions $R_1, R_2, ..., R_J$.
- For each observation in region R_j , compute the mean of the response values:

$$\hat{y}_{R_j} = \frac{1}{\# R_j} \sum_{i \in R_j} y_i$$







Tree-based methods: application to economics

Tree-based methods

Regression trees

Building a regression tree

Q: How the regions are constructed?







Regression trees

Building a regression tree

Q: How the regions are constructed?

A: Using a top-down, greedy approach: recursive binary splitting







Q: How the regions are constructed ?

A: Using a top-down, greedy approach: recursive binary splitting

<u>Goal</u>: find regions $R_1, ..., R_J$ that **minimize the residual sum of squares**, defined by:

$$RSS = \sum_{j=1}^{J} \sum_{i \in R_j} (y_i - \hat{y}_{R_j})^2$$







Q: How the regions are constructed ?

A: Using a top-down, greedy approach: recursive binary splitting

<u>Goal</u>: find regions $R_1, ..., R_J$ that **minimize the residual sum of squares**, defined by:

$$RSS = \sum_{j=1}^{J} \sum_{i \in R_j} (y_i - \hat{y}_{R_j})^2$$

Note: RSS is also called the training error







Tree-based methods: application to economics

Tree-based methods

Regression trees

Building a regression tree

Recursive binary splitting:







Regression trees

Building a regression tree

Recursive binary splitting:

• Consider the **feature** X_j







Regression trees

Building a regression tree

Recursive binary splitting:

- Consider the **feature** X_i
- Select a **cutpoint** $s \in \mathcal{S}(X_j)$







- Tree-based methods
- Regression trees

Recursive binary splitting:

- Consider the feature X_i
- Select a **cutpoint** $s \in \mathcal{S}(X_j)$
- **Split** the feature space in two regions R_l and R_r such that:

$$R_l(j,s) = \{X | X_j < s\} \text{ and } R_r(j,s) = \{X | X_j \ge s\}$$







Recursive binary splitting:

- Consider the feature X_i
- Select a **cutpoint** $s \in \mathcal{S}(X_j)$
- **Split** the feature space in two regions R_l and R_r such that:

$$R_{I}(j,s) = \{X|X_{j} < s\} \text{ and } R_{r}(j,s) = \{X|X_{j} \ge s\}$$

Finally we keep the pair (j, s) that **minimize**

$$\sum_{i:x_{i}\in R_{l}(j,s)} (y_{i} - \hat{y}_{R_{l}})^{2} + \sum_{i:x_{i}\in R_{r}(j,s)} (y_{i} - \hat{y}_{R_{r}})^{2}$$







Regression trees

Building a regression tree

This process is repeated for the new regions obtained







Tree-based methods

Regression trees

Building a regression tree

This process is repeated for the new regions obtained

Continues until a **stopping criterion** (e.g minimum size of a region) is verified







Tree-based methods
Regression trees

Building a regression tree

This process is repeated for the new regions obtained

Continues until a **stopping criterion** (e.g minimum size of a region) is verified

The resulting tree is call the maximal tree







Regression trees

Pruning the maximal tree

The maximal tree might be too complex (in terms of depth)







Tree-based methods
Regression trees

Pruning the maximal tree

The maximal tree might be too complex (in terms of depth)

A smaller tree with less splits (regions): better interpretation, lower variance







Tree-based methods

Regression trees

Pruning the maximal tree

The maximal tree might be too complex (in terms of depth)

A smaller tree with less splits (regions): better interpretation, lower variance

Pruning consists in growing a very large tree T_0 and reduce it back to obtain a **subtree**







Regression trees

Pruning the maximal tree

Cost complexity pruning or Weakest link pruning







Regression trees

Pruning the maximal tree

Cost complexity pruning or Weakest link pruning

We define a measure that take into account both training error and tree complexity







Pruning the maximal tree

Cost complexity pruning or Weakest link pruning

We define a measure that take into account both training error and tree complexity

<u>Goal</u>: For a given value α (**complexity parameter**), find a subtree $T \subset T_0$ that minimizes

$$\sum_{m=1}^{|T|} \sum_{x_i \in R_m} (y_i - \hat{y}_{R_m})^2 + \alpha |T|$$







Tree-based methods

Regression trees

Example: Predicting Baseball Players' Salaries

<u>Data</u>: **Hitters** dataset (Major League Baseball Data from the 1986 and 1987 seasons) containing 322 observations of 20 features.







- Tree-based methods
 - Regression trees

Example: Predicting Baseball Players' Salaries

<u>Data</u>: **Hitters** dataset (Major League Baseball Data from the 1986 and 1987 seasons) containing 322 observations of 20 features.

<u>Goal</u>: Predict a baseball player's **Salary** based on **Years** (number of years played in major leagues) and **Hits** (number of hits made in the previous season).







- Tree-based methods
- Regression trees

Name	Years	Hits	Salary
Alan Ashby	14	81	475.0
Alvin Davis	3	130	480.0
Andre Dawson	11	141	500.0
Andres Galarraga	2	87	91.5
Alfredo Griffin	11	169	750.0

Figure: A sample of baseball players





- Tree-based methods
 Regression trees
- Name Years Hits Salary Alan Ashby 81 475.0 14 Alvin Davis 3 130 480.0 Andre Dawson 11 141 500.0 Andres Galarraga 2 87 91.5 Alfredo Griffin 11 169 750.0

Figure: A sample of baseball players

We denote:

- X₁: Years (exogeneous)
- X_2 : Hits (exogeneous)
- Y: log(Salary) (endogeneous)

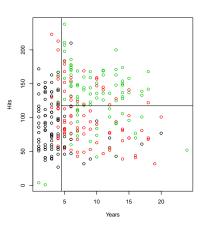


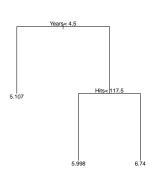




Tree-based methods

Regression trees











Tree-based methods

Classification trees

Classification tree

A classification tree is similar to a regression tree







Classification tree

A classification tree is similar to a regression tree

Used to predict a **qualitative** response variable:

$$Y \in \{0,...,K\}, K \in \mathbb{N}^*$$







Classification tree

A classification tree is similar to a regression tree

Used to predict a **qualitative** response variable:

$$Y \in \{0,...,K\}, K \in \mathbb{N}^*$$

Assign to each region R_j the **most commonly occurring class** of observations in R_j







Classification tree

A classification tree is similar to a regression tree

Used to predict a **qualitative** response variable:

$$Y \in \{0,...,K\}, K \in \mathbb{N}^*$$

Assign to each region R_j the ${\bf most}$ commonly occurring class of observations in R_j

<u>Problem</u>: RSS cannot be used in classification: an alternative to RSS is the **classification error rate**







Tree-based methods: application to economics

Tree-based methods

Classification trees

Classification error rate

The classification error rate in a given region is the proportion of training observations in that region that do not belong to the most common class:







Classification error rate

The classification error rate in a given region is the proportion of training observations in that region that do not belong to the most common class:

$$E = 1 - \max_{k} (\hat{p}_{mk})$$







- Tree-based methods
 - Classification trees

Classification error rate

The classification error rate in a given region is the proportion of training observations in that region that do not belong to the most common class:

$$E=1-\max_k(\hat{p}_{mk})$$

Here, \hat{p}_{mk} is the proportion of training observations in the m^{th} region that are from the k^{th} class







Tree-based methods

Classification trees

Classification error rate

The classification error rate in a given region is the proportion of training observations in that region that do not belong to the most common class:

$$E=1-\max_k(\hat{p}_{mk})$$

Here, \hat{p}_{mk} is the proportion of training observations in the m^{th} region that are from the k^{th} class

Note: in practice, two other measures are used







Tree-based methods

Classification trees

Gini index

The Gini index is defined as follows:

$$G = \sum_{k=1}^K \hat{p}_{mk}(1-\hat{p}_{mk})$$







- Tree-based methods

Classification trees

Gini index

The Gini index is defined as follows:

$$G = \sum_{k=1}^K \hat{p}_{mk}(1 - \hat{p}_{mk})$$

This is a measure of total variance across the K classes







Tree-based methods

Classification trees

Gini index

The Gini index is defined as follows:

$$G = \sum_{k=1}^K \hat{p}_{mk} (1 - \hat{p}_{mk})$$

This is a measure of total variance across the K classes

The Gini index is a measure of **purity**: small values indicate that a node contains a predominant class





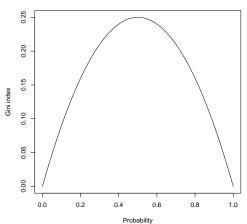


Tree-based methods

Classification trees

Gini index











Tree-based methods

Classification trees

Cross-entropy

An alternative to the Gini index

$$D = -\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}$$







Tree-based methods

Classification trees

Cross-entropy

An alternative to the Gini index

$$D = -\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}$$

This is also a measure of purity: small values indicate that a node is **pure**







Tree-based methods

Classification trees

Cross-entropy

An alternative to the Gini index

$$D = -\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}$$

This is also a measure of purity: small values indicate that a node is **pure**

Note: Gini index and cross-entropy are similar numerically





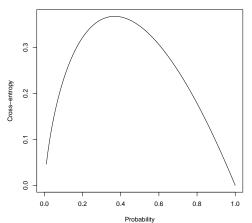


Tree-based methods

└─ Classification trees

Cross-entropy











Classification trees

Example: predicting heart disease

<u>Data</u>: **Heart** dataset containing 303 observations of 14 features.







Tree-based methods

Classification trees

Example: predicting heart disease

<u>Data</u>: **Heart** dataset containing 303 observations of 14 features.

<u>Goal</u>: Predict the presence of heart disease HD based on different predictors such as Age, Sex, Chol (a cholesterol measurement)...







- Tree-based methods
 - Classification trees

Age	Sex	Chestpain	 HD
63	1	typical	 No
67	1	asymptomatic	 Yes
67	1	asymptomatic	 Yes
37	1	nonanginal	 No
41	0	nontypical	 No

Figure: A sample of patients





- Tree-based methods
 - Classification trees

Age	Sex	Chestpain	 HD
63	1	typical	 No
67	1	asymptomatic	 Yes
67	1	asymptomatic	 Yes
37	1	nonanginal	 No
41	0	nontypical	 No

Figure: A sample of patients

We denote:

- X_1 : Age (exogeneous)
- X₂: Sex (exogeneous)
- •
- Y: HD (endogeneous)



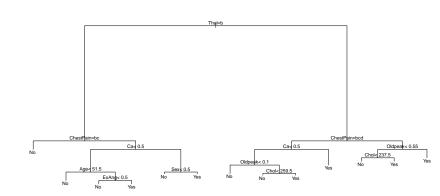




Tree-based methods: application to economics

Tree-based methods

Classification trees





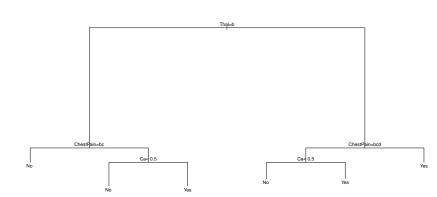




Tree-based methods: application to economics

Tree-based methods

Classification trees









Classification trees

Trees: pros and cons

Pros:

- Easy to use
- Help decision making
- Graphical, interpretable
- Deal with both quantitative and qualitative features

Cons:

- Not the best method in terms of prediction accuracy
- Trees are unstable







- Advanced tree-based methods

3 Advanced tree-based methods
Bagging and Random Forest
Clustering using binary trees
Variable importance







Advanced tree-based methods

Bagging and Random Forest

Bagging

Bootstrap aggregation (or **bagging**) is a procedure for reducing the variance of a statistial learning method







- Advanced tree-based methods
 - ☐ Bagging and Random Forest

Bagging

Bootstrap aggregation (or **bagging**) is a procedure for reducing the variance of a statistial learning method

Given a set of n independent observations $Z_1,...,Z_n$ each with variance σ^2 , the variance of the mean \bar{Z} is $\frac{\sigma^2}{n}$







- Advanced tree-based methods
 - ☐ Bagging and Random Forest

Bagging

Bootstrap aggregation (or **bagging**) is a procedure for reducing the variance of a statistial learning method

Given a set of n independent observations $Z_1,...,Z_n$ each with variance σ^2 , the variance of the mean \bar{Z} is $\frac{\sigma^2}{n}$

Averaging a set of obervations reduces variance







- Advanced tree-based methods

Bagging and Random Forest

Bagging

Idea:

• Calculate B predictions denoted $\hat{f}^1(x), \hat{f}^2(x), ..., \hat{f}^B(x)$ using B separate training sets





Advanced tree-based methods

☐ Bagging and Random Forest

Bagging

Idea:

- Calculate B predictions denoted $\hat{f}^1(x), \hat{f}^2(x), ..., \hat{f}^B(x)$ using B separate training sets
- Average the B predictions to obtain a single low-variance statistical learning model:

$$\hat{f}_{avg}(x) = \frac{1}{B} \sum_{b=1}^{B} \hat{f}^b(x)$$







Bagging

Idea:

- Calculate B predictions denoted $\hat{f}^1(x), \hat{f}^2(x), ..., \hat{f}^B(x)$ using B separate training sets
- Average the B predictions to obtain a single low-variance statistical learning model:

$$\hat{f}_{avg}(x) = \frac{1}{B} \sum_{b=1}^{B} \hat{f}^b(x)$$

 <u>Problem</u>: In practice, we do not have access to multiple training sets







-Advanced tree-based methods

Bagging and Random Forest

Bagging

Solution:

• Generate *B* bootstrapped training datasets







Advanced tree-based methods

Bagging and Random Forest

Bagging

Solution:

- Generate B bootstrapped training datasets
- Train a model (a tree) on the b^{th} bootstrapped training dataset in ordre to get $\hat{f}*b(x)$







Bagging

Solution:

- Generate B bootstrapped training datasets
- Train a model (a tree) on the b^{th} bootstrapped training dataset in ordre to get $\hat{f}*b(x)$
- Average all the predictions:

$$\hat{f}_{bag}(x) = \frac{1}{B} \sum_{b=1}^{B} \hat{f} * b(x)$$







- Advanced tree-based methods

Bagging and Random Forest

Random forest

 RF is an improvement over bagged trees, using a "trick" that decorrelated the bootstrapped trees







- Advanced tree-based methods
 - Bagging and Random Forest

Random forest

- RF is an improvement over bagged trees, using a "trick" that decorrelated the bootstrapped trees
- A random sample of m predictors is chosen among the full set of p predictors at each split of the tree







Random forest

- RF is an improvement over bagged trees, using a "trick" that decorrelated the bootstrapped trees
- A random sample of m predictors is chosen among the full set of p predictors at each split of the tree
- Typically, we choose $m=\sqrt{p}$, useful when we have a high number of correlated predictors







- Advanced tree-based methods

Clustering using binary trees

Unsupervised learning

Two issues in unsupervised learning: Clustering and Density estimation







- Advanced tree-based methods

Clustering using binary trees

Unsupervised learning

- Two issues in unsupervised learning: Clustering and Density estimation
- We have no endogeneous feature Y







- Advanced tree-based methods

Clustering using binary trees

Unsupervised learning

- Two issues in unsupervised learning: Clustering and Density estimation
- We have no endogeneous feature Y
- We focus on clustering



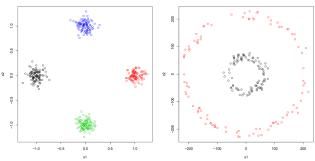




- Advanced tree-based methods
- Clustering using binary trees

Unsupervised learning

- Two issues in unsupervised learning: Clustering and Density estimation
- We have no endogeneous feature Y
- We focus on clustering









-Advanced tree-based methods

Clustering using binary trees

Clustering

Suppose we have a set of training observations $\{X_i\}$, i=1,...,n, we try to find a **partition** of this set in K clusters, minimizing **within-cluster heterogeneity** and maximizing **between-cluster heterogeneity**. There are three main approaches:







- Advanced tree-based methods
 - Clustering using binary trees

Suppose we have a set of training observations $\{X_i\}$, i=1,...,n, we try to find a **partition** of this set in K clusters, minimizing **within-cluster heterogeneity** and maximizing **between-cluster heterogeneity**. There are three main approaches:

• hierarchical methods (e.g HCA)







- Advanced tree-based methods
 - Clustering using binary trees

Suppose we have a set of training observations $\{X_i\}$, i=1,...,n, we try to find a **partition** of this set in K clusters, minimizing **within-cluster heterogeneity** and maximizing **between-cluster heterogeneity**. There are three main approaches:

- hierarchical methods (e.g HCA)
- partitional methods (e.g K-means)







- Advanced tree-based methods
 - Clustering using binary trees

Suppose we have a set of training observations $\{X_i\}$, i=1,...,n, we try to find a **partition** of this set in K clusters, minimizing **within-cluster heterogeneity** and maximizing **between-cluster heterogeneity**. There are three main approaches:

- hierarchical methods (e.g HCA)
- partitional methods (e.g K-means)
- density-based methods







- Advanced tree-based methods
 - Clustering using binary trees

Suppose we have a set of training observations $\{X_i\}$, i=1,...,n, we try to find a **partition** of this set in K clusters, minimizing **within-cluster heterogeneity** and maximizing **between-cluster heterogeneity**. There are three main approaches:

- hierarchical methods (e.g HCA)
- partitional methods (e.g K-means)
- density-based methods

Classical problems:







- -Advanced tree-based methods
 - Clustering using binary trees

Suppose we have a set of training observations $\{X_i\}$, i=1,...,n, we try to find a **partition** of this set in K clusters, minimizing **within-cluster heterogeneity** and maximizing **between-cluster heterogeneity**. There are three main approaches:

- hierarchical methods (e.g HCA)
- partitional methods (e.g K-means)
- density-based methods

Classical problems:

- Measure the **performance** of a partition
- Choose the optimal value of K, the **number of clusters**







- Advanced tree-based methods

Clustering using binary trees

Clustering using unsupervised binary trees

CUBT is a top-down hierarchical clustering methods that works in **3 steps**:







- Advanced tree-based methods

Clustering using binary trees

Clustering using unsupervised binary trees

CUBT is a top-down hierarchical clustering methods that works in **3 steps**:

• growing the maximal tree: recursive binary partitioning







- Advanced tree-based methods

Clustering using binary trees

Clustering using unsupervised binary trees

CUBT is a top-down hierarchical clustering methods that works in **3 steps**:

- growing the maximal tree: recursive binary partitioning
- pruning the tree (dissimilarity-based pruning)







Clustering using binary trees

Clustering using unsupervised binary trees

CUBT is a top-down hierarchical clustering methods that works in **3 steps**:

- growing the maximal tree: recursive binary partitioning
- pruning the tree (dissimilarity-based pruning)
- joining the leaves of the tree (alternative pruning)







- Advanced tree-based methods

Clustering using binary trees

Similarities with CART







- Advanced tree-based methods

Clustering using binary trees

Similarities with CART

CUBT has many similarities with CART:

Efficiency







- Advanced tree-based methods

Clustering using binary trees

Similarities with CART

- Efficiency
- Flexibility







- Advanced tree-based methods

Clustering using binary trees

Similarities with CART

- Efficiency
- Flexibility
- Interpretability







- Advanced tree-based methods

Clustering using binary trees

Similarities with CART

- Efficiency
- Flexibility
- Interpretability
- Good convergence properties







- Advanced tree-based methods

Clustering using binary trees

Step 1: Growing the maximal tree

Let t be a tree node containing a set of observations in \mathbb{R}^p .







- Advanced tree-based methods

Clustering using binary trees

Step 1: Growing the maximal tree

Let t be a tree node containing a set of observations in \mathbb{R}^p . The **child nodes** of t are denoted t_L and t_R , defined as follows:







- Advanced tree-based methods

Clustering using binary trees

Step 1: Growing the maximal tree

Let t be a tree node containing a set of observations in \mathbb{R}^p . The **child nodes** of t are denoted t_L and t_R , defined as follows:

$$t_L = \{x \in \mathbb{R}^p | x_j \le a\}$$
 and $t_R = \{x \in \mathbb{R}^p | x_j > a\}$







Let t be a tree node containing a set of observations in \mathbb{R}^p . The **child nodes** of t are denoted t_L and t_R , defined as follows:

$$t_L = \{x \in \mathbb{R}^p | x_j \le a\}$$
 and $t_R = \{x \in \mathbb{R}^p | x_j > a\}$

Let $X_t = \{X | X \in t\}$, $\alpha_t = P(X \in t)$ and R(t) a heterogeneity measure (**deviance**) of t, defined as:







Let t be a tree node containing a set of observations in \mathbb{R}^p . The **child nodes** of t are denoted t_L and t_R , defined as follows:

$$t_L = \{x \in \mathbb{R}^p | x_j \le a\}$$
 and $t_R = \{x \in \mathbb{R}^p | x_j > a\}$

Let $X_t = \{X | X \in t\}$, $\alpha_t = P(X \in t)$ and R(t) a heterogeneity measure (**deviance**) of t, defined as:

$$R(t) = \alpha_t trace(cov(X_t))$$







Let t be a tree node containing a set of observations in \mathbb{R}^p . The **child nodes** of t are denoted t_L and t_R , defined as follows:

$$t_L = \{x \in \mathbb{R}^p | x_j \le a\}$$
 and $t_R = \{x \in \mathbb{R}^p | x_j > a\}$

Let $X_t = \{X | X \in t\}$, $\alpha_t = P(X \in t)$ and R(t) a heterogeneity measure (**deviance**) of t, defined as:

$$R(t) = \alpha_t trace(cov(X_t))$$

The **best split** of t is defined by the pair $(j, a) \in \{1, ...p\} \times \mathbb{R}$ maximizing

$$\Delta(t,j,a) = R(t) - R(t_L) - R(t_R)$$







- Advanced tree-based methods

Clustering using binary trees

Step 1: Growing the maximal tree

We denote S the initial training dataset, each node t is split recursively until the following **stopping criteria** are verified:







Clustering using binary trees

Step 1: Growing the maximal tree

We denote S the initial training dataset, each node t is split recursively until the following **stopping criteria** are verified:

• All observations in t are the same







We denote S the initial training dataset, each node t is split recursively until the following **stopping criteria** are verified:

- All observations in t are the same
- There are less than *minsize* observations in *t*







Step 1: Growing the maximal tree

We denote S the initial training dataset, each node t is split recursively until the following **stopping criteria** are verified:

- All observations in t are the same
- There are less than *minsize* observations in t
- $\Delta(t, j, a) < mindev \times R(S)$







Step 1: Growing the maximal tree

We denote S the initial training dataset, each node t is split recursively until the following **stopping criteria** are verified:

- All observations in t are the same
- There are less than minsize observations in t
- $\Delta(t, j, a) < mindev \times R(S)$

The clustering **tree** represents the **partition**.







Step 1: Growing the maximal tree

We denote S the initial training dataset, each node t is split recursively until the following **stopping criteria** are verified:

- All observations in t are the same
- There are less than *minsize* observations in *t*
- $\Delta(t, j, a) < mindev \times R(S)$

The clustering **tree** represents the **partition**. Each **leaf** represents a **cluster**.







- Advanced tree-based methods

Clustering using binary trees

Step 2: Pruning the tree

We denote t_L and t_R the leaves obtained by splitting t.







- Advanced tree-based methods

Clustering using binary trees

Step 2: Pruning the tree

We denote t_L and t_R the leaves obtained by splitting t.

Pruning criterion

If $d^{\delta}(L,R) \leq mindist$ then t_L and t_R are aggregated







Advanced tree-based methods

Clustering using binary trees

Step 2: Pruning the tree

We denote t_L and t_R the leaves obtained by splitting t.

Pruning criterion

If $d^{\delta}(L,R) \leq mindist$ then t_L and t_R are aggregated $d^{\delta}(L,R)$ is an empirical dissimilarity measure between t_L and t_R :







Step 2: Pruning the tree

We denote t_L and t_R the leaves obtained by splitting t.

Pruning criterion

If $d^{\delta}(L,R) \leq mindist$ then t_L and t_R are aggregated $d^{\delta}(L,R)$ is an empirical dissimilarity measure between t_L and t_R :

$$d^{\delta}(L,R) = \max(\bar{d}_L^{\delta},\bar{d}_R^{\delta})$$







Step 2: Pruning the tree

We denote t_L and t_R the leaves obtained by splitting t.

Pruning criterion

If $d^{\delta}(L,R) \leq mindist$ then t_L and t_R are aggregated $d^{\delta}(L,R)$ is an empirical dissimilarity measure between t_L and t_R :

$$d^{\delta}(L,R) = \max(\bar{d}_L^{\delta},\bar{d}_R^{\delta})$$

where $\forall \delta \in [0,1]$







└Clustering using binary trees

Step 2: Pruning the tree

We denote t_L and t_R the leaves obtained by splitting t.

Pruning criterion

If $d^{\delta}(L,R) \leq mindist$ then t_L and t_R are aggregated $d^{\delta}(L,R)$ is an empirical dissimilarity measure between t_L and t_R :

$$d^{\delta}(L,R) = \max(\bar{d}_L^{\delta},\bar{d}_R^{\delta})$$

where $\forall \delta \in [0,1]$

$$ar{d}_L^\delta = rac{1}{\delta n_L} \sum_{i=1}^{\delta n_L} d_i \ ext{and} \ ar{d}_R^\delta = rac{1}{\delta n_R} \sum_{i=1}^{\delta n_R} d_i$$







- Advanced tree-based methods

Clustering using binary trees

Step 2: Dissimilarity measure

$$\forall X_i \in t_R \text{ and } X_j \in t_L \text{ we have:}$$







- Advanced tree-based methods

Clustering using binary trees

Step 2: Dissimilarity measure

$$\forall X_i \in t_R \text{ and } X_j \in t_L \text{ we have:}$$

$$ilde{d}_i = \min_{x \int_R} d(X_i, x) \text{ and } ilde{d}_j = \min_{x \int_L} d(x, X_j)$$







Clustering using binary trees

Step 2: Dissimilarity measure

$$\forall X_i \in t_R \text{ and } X_j \in t_L \text{ we have:}$$

$$ilde{d}_i = \min_{x \int_R} d(X_i, x) \text{ and } ilde{d}_j = \min_{x \int_L} d(x, X_j)$$

and their ordered versions $\{d_i\}$ and $\{d_j\}$,







Step 2: Dissimilarity measure

 $\forall X_i \in t_R \text{ and } X_j \in t_L \text{ we have:}$

$$ilde{d}_i = \min_{x \int_R} d(X_i, x) ext{ and } ilde{d}_j = \min_{x \int_L} d(x, X_j)$$

and their ordered versions $\{d_i\}$ and $\{d_j\}$, where d(X,y) is the Euclidean distance

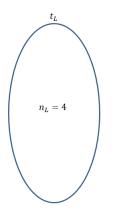


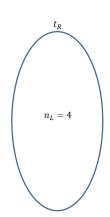




Advanced tree-based methods

Clustering using binary trees





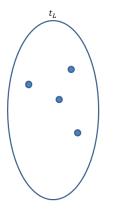


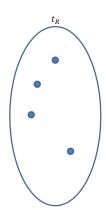




Advanced tree-based methods

Clustering using binary trees





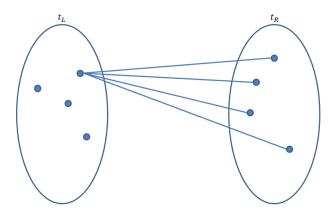






-Advanced tree-based methods

Clustering using binary trees



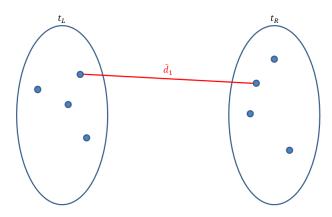






-Advanced tree-based methods

Clustering using binary trees



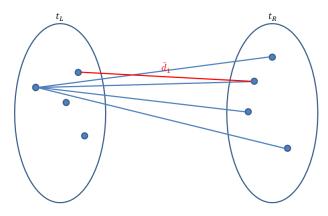






Advanced tree-based methods

Clustering using binary trees



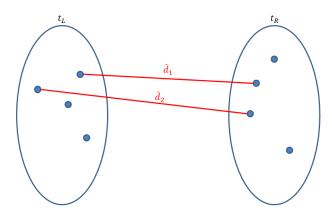






Advanced tree-based methods

Clustering using binary trees



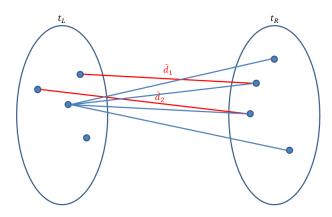






Advanced tree-based methods

Clustering using binary trees



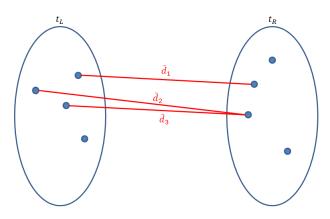






Advanced tree-based methods

Clustering using binary trees



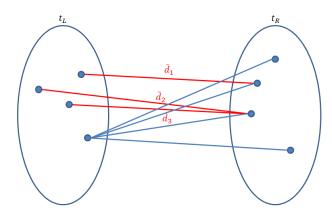






Advanced tree-based methods

Clustering using binary trees



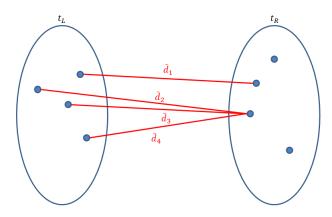






Advanced tree-based methods

Clustering using binary trees









- Advanced tree-based methods

Clustering using binary trees

Step 3: Joining the leaves

We aggregate leaves that are not issued from a same parent







- Advanced tree-based methods

Clustering using binary trees

Step 3: Joining the leaves

We aggregate leaves that are not issued from a same parent

Two joining criteria

Leaves are compared using:







Clustering using binary trees

Step 3: Joining the leaves

We aggregate leaves that are not issued from a same parent

Two joining criteria

Leaves are compared using:





Clustering using binary trees

Step 3: Joining the leaves

We aggregate leaves that are not issued from a same parent

Two joining criteria

Leaves are compared using:





Step 3: Joining the leaves

We aggregate leaves that are not issued from a same parent

Two joining criteria

Leaves are compared using:

Let N_L be the total number of leaves and K the expected number of classes.







Step 3: Joining the leaves

We aggregate leaves that are not issued from a same parent

Two joining criteria

Leaves are compared using:

Let N_L be the total number of leaves and K the expected number of classes. $\forall (L,R) \in \{1,...,N_L\}$ and $L \neq R$ we have $(\tilde{L},\tilde{R}) = argmin_{L,R}\Delta(t_L,t_R)$







Step 3: Joining the leaves

We aggregate leaves that are not issued from a same parent

Two joining criteria

Leaves are compared using:

Let N_i be the total number of leaves and K the expected number of classes. $\forall (L, R) \in \{1, ..., N_L\}$ and $L \neq R$ we have $(\tilde{L}, \tilde{R}) = \operatorname{argmin}_{LR} \Delta(t_L, t_R)$

Joining the leaves

 $t_{\tilde{I}}$ and $t_{\tilde{R}}$ are replaced by their union $t_{\tilde{I}} \cup t_{\tilde{R}}$ and $N_L = N_L - 1$. Stop when $N_I = K$.







- Advanced tree-based methods

Clustering using binary trees

CUBT: pros and cons

Pros:

- Decisional method
- Interpretable
- Extensions to other types of data
- Adapted to parallel computing
- Partition of the feature space, not only the training dataset

Cons:

- Same as CART
- Trees are unstable







- Advanced tree-based methods

└─Variable importance

Motivation and objectives

Motivation







- Advanced tree-based methods

└─Variable importance

Motivation and objectives

Motivation

Feature selection







- Advanced tree-based methods

└─Variable importance

Motivation and objectives

Motivation

- Feature selection
- Dimension reduction







Advanced tree-based methods

└─Variable importance

Motivation and objectives

Motivation

- Feature selection
- Dimension reduction
- Missing data







Advanced tree-based methods

└─Variable importance

Motivation and objectives

Motivation

- Feature selection
- Dimension reduction
- Missing data

Objectives







- Advanced tree-based methods

└─Variable importance

Motivation and objectives

Motivation

- Feature selection
- Dimension reduction
- Missing data

Objectives

Define variable importance in CUBT







Advanced tree-based methods

└Variable importance

Motivation and objectives

Motivation

- Feature selection
- Dimension reduction
- Missing data

Objectives

- Define variable importance in CUBT
- Analyze its stability







- Advanced tree-based methods

└Variable importance

Motivation and objectives

Motivation

- Feature selection
- Dimension reduction
- Missing data

Objectives

- Define variable importance in CUBT
- Analyze its stability
- Compare to other methods



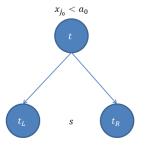


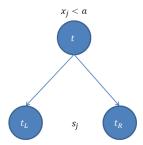


- Advanced tree-based methods
 - └─Variable importance

Competitive splits

To compute the importance of a feature j, we define the **competitive split** of a feature j_0 in a node t.











-Advanced tree-based methods

└Variable importance

Competitive splits

The probability that an observation is sent to the **left node** for both splits is







Advanced tree-based methods

└Variable importance

Competitive splits

The probability that an observation is sent to the **left node** for both splits is

$$p(t_L \cap t'_L) = \frac{\#\{t_L \cap t'_L\}}{n_t}$$







Competitive splits

The probability that an observation is sent to the **left node** for both splits is

$$p(t_L \cap t'_L) = \frac{\#\{t_L \cap t'_L\}}{n_t}$$

Given a observation is in t, the probability that both splits sent it to the left is







Uariable importance

Competitive splits

The probability that an observation is sent to the **left node** for both splits is

$$p(t_L \cap t'_L) = \frac{\#\{t_L \cap t'_L\}}{n_t}$$

Given a observation is in t, the probability that both splits sent it to the left is

$$p_{LL}(s,s_j) = \frac{p(t_L \cap t'_L)}{p(t)}$$







Competitive splits

The probability that an observation is sent to the **left node** for both splits is

$$p(t_L \cap t'_L) = \frac{\#\{t_L \cap t'_L\}}{n_t}$$

Given a observation is in t, the probability that both splits sent it to the left is

$$p_{LL}(s,s_j) = \frac{p(t_L \cap t'_L)}{p(t)}$$

 p_{RR} can be defined equivalently







- Advanced tree-based methods

└Variable importance

Surrogate splits and variable importance

We define an association measure between s_j and s







- Advanced tree-based methods

└Variable importance

Surrogate splits and variable importance

We define an association measure between s_j and s

$$p(s,s_j)=p_{LL}+p_{RR}$$







- Advanced tree-based methods

UVariable importance

Surrogate splits and variable importance

We define an association measure between s_j and s

$$p(s,s_j)=p_{LL}+p_{RR}$$

 \tilde{s}_j is a surrogate split of s if







Advanced tree-based methods

└Variable importance

Surrogate splits and variable importance

We define an association measure between s_j and s

$$p(s,s_j)=p_{LL}+p_{RR}$$

 \tilde{s}_j is a surrogate split of s if $p(s, \tilde{s}_j) = max_{s_j}p(s, s_j)$







UVariable importance

Surrogate splits and variable importance

We define an association measure between s_j and s

$$p(s,s_j) = p_{LL} + p_{RR}$$

 \tilde{s}_j is a **surrogate split** of s if $p(s, \tilde{s}_j) = max_{s_j}p(s, s_j)$ The importance of the variable j is given by







Surrogate splits and variable importance

We define an association measure between s_i and s

$$p(s,s_j)=p_{LL}+p_{RR}$$

 \tilde{s}_j is a **surrogate split** of s if $p(s, \tilde{s}_j) = max_{s_j}p(s, s_j)$ The importance of the variable j is given by

$$Imp(X_j) = \sum_t \Delta(R(\tilde{s}_j, t))$$







Surrogate splits and variable importance

We define an association measure between s_i and s

$$p(s,s_j) = p_{LL} + p_{RR}$$

 \tilde{s}_j is a **surrogate split** of s if $p(s, \tilde{s}_j) = max_{s_j}p(s, s_j)$ The importance of the variable j is given by

$$Imp(X_j) = \sum_t \Delta(R(\tilde{s}_j, t))$$

which is the **loss of deviance** induced if each node is replaced by the surrogate split defined on X_i







- Advanced tree-based methods

└─Variable importance

Conclusion

CUBT is an interpretable clustering method







Advanced tree-based methods

└Variable importance

Conclusion

- CUBT is an interpretable clustering method
- Measure of variable importance in CUBT







- Advanced tree-based methods

└Variable importance

Conclusion

- CUBT is an interpretable clustering method
- Measure of variable importance in CUBT
- Heuristics have been proposed for tuning the method







└Variable importance

Conclusion

- CUBT is an interpretable clustering method
- Measure of variable importance in CUBT
- Heuristics have been proposed for tuning the method
- Stability of variable importance







Applications to Economics: Causal Trees

4 Applications to Economics: Causal Trees







Recursive partitioning for heterogeneous causal effect . Susan Athey and Guido Imbens (2016). In PNAS.







Recursive partitioning for heterogeneous causal effect . Susan Athey and Guido Imbens (2016). In PNAS.

• Estimating heterogeneity in causal effects







Recursive partitioning for heterogeneous causal effect . Susan Athey and Guido Imbens (2016). In PNAS.

- Estimating heterogeneity in causal effects
- Evaluating the differences in treatment effects across subsets of population







Recursive partitioning for heterogeneous causal effect . Susan Athey and Guido Imbens (2016). In PNAS.

- Estimating heterogeneity in causal effects
- Evaluating the differences in treatment effects across subsets of population
- Using recursive binary partitioning







Recursive partitioning for heterogeneous causal effect . Susan Athey and Guido Imbens (2016). In PNAS.

- Estimating heterogeneity in causal effects
- Evaluating the differences in treatment effects across subsets of population
- Using recursive binary partitioning

This approach is based on regression trees, modified to take into account the treatment effects in causal models







• We have N units, indexed by i = 1, ..., N







- We have *N* units, indexed by i = 1, ..., N
- We suppose the existence of **potential outcomes** for each unit, (Y_i(0), Y_i(1)) (Rubin Causal Model)







- We have *N* units, indexed by i = 1, ..., N
- We suppose the existence of **potential outcomes** for each unit, $(Y_i(0), Y_i(1))$ (Rubin Causal Model)
- Difference in potential outcomes, $\tau_i = Y_i(1) Y_i(0)$





- We have *N* units, indexed by i = 1, ..., N
- We suppose the existence of **potential outcomes** for each unit, $(Y_i(0), Y_i(1))$ (Rubin Causal Model)
- Difference in potential outcomes, $\tau_i = Y_i(1) Y_i(0)$
- $W_i \in \{0,1\}$, binary indicator of the treatment (0 for control, 1 for treatment)





- We have *N* units, indexed by i = 1, ..., N
- We suppose the existence of **potential outcomes** for each unit, $(Y_i(0), Y_i(1))$ (Rubin Causal Model)
- Difference in potential outcomes, $\tau_i = Y_i(1) Y_i(0)$
- $W_i \in \{0,1\}$, binary indicator of the treatment (0 for control, 1 for treatment)
- The outcome is

$$Y_i^{obs} = Y_i(W_i) = \begin{cases} Y_i(0) & \text{if } W_i = 0 \\ Y_i(1) & \text{if } W_i = 1 \end{cases}$$







Let X_i be a **vector of features** (covariates, variables), not affected by the treatment







Let X_i be a **vector of features** (covariates, variables), not affected by the treatment

We assume **unconfoundedness**, $W_i(Y_i(0), Y_i(1))|X_i$







Let X_i be a **vector of features** (covariates, variables), not affected by the treatment

We assume **unconfoundedness**, $W_i(Y_i(0), Y_i(1))|X_i(0)|$

We try to estimate the **conditional average treatment effect** (CATE)

$$\tau(x) = \mathbb{E}[Y_i(1) - Y_i(0)|X_i = x]$$







Honest estimation

Causal trees are based on CART, the difference is in the estimation:







Honest estimation

Causal trees are based on CART, the difference is in the estimation:

• Estimation CATE rather than predicting outcomes







Causal trees are based on CART, the difference is in the estimation:

- Estimation CATE rather than predicting outcomes
- "Honest" estimation: use separate datasets for constructing the partition (the regions) and estimating the effects within the leaves







Causal trees are based on CART, the difference is in the estimation:

- Estimation CATE rather than predicting outcomes
- "Honest" estimation: use separate datasets for constructing the partition (the regions) and estimating the effects within the leaves
- In CART, the estimation is "adaptive" (same dataset)







Applications to Economics: Causal Trees

Honest estimation

Suppose the feature space is the union of two subsamples L and R







Suppose the feature space is the union of two subsamples L and R

Given a sample S, the average outcomes in the two subsamples are \bar{Y}_L and \bar{Y}_R





Suppose the feature space is the union of two subsamples L and R

Given a sample S, the average outcomes in the two subsamples are \bar{Y}_L and \bar{Y}_R

Algorithm: Split the feature space if the difference in average outcomes exceeds a threshold c:







Suppose the feature space is the union of two subsamples L and R

Given a sample S, the average outcomes in the two subsamples are \bar{Y}_L and \bar{Y}_R

Algorithm: Split the feature space if the difference in average outcomes exceeds a threshold c:

$$\pi(S) = \begin{cases} \{\{L, R\}\} & \text{if } \bar{Y}_L - \bar{Y}_R \le c \\ \{\{L\}, \{R\}\} & \text{if } \bar{Y}_L - \bar{Y}_R > c \end{cases}$$







Applications to Economics: Causal Trees

Honest estimation

• Let Π a **tree** defining a partition on the feature space.







- Let Π a **tree** defining a partition on the feature space.
- Let $I(x,\Pi)$ the leaf $I \in \Pi$ such that $x \in I$







- Let Π a **tree** defining a partition on the feature space.
- Let $I(x,\Pi)$ the leaf $I \in \Pi$ such that $x \in I$
- The estimated outcomes is







- Let Π a **tree** defining a partition on the feature space.
- Let $I(x,\Pi)$ the leaf $I \in \Pi$ such that $x \in I$
- The estimated outcomes is

$$\hat{\mu}(x,S,\Pi) = \frac{1}{\#(i \in S : X_i \in I(x,\Pi))} \sum_{i \in S: X_i \in I(x,\Pi)} Y_i$$







Honest target

The goal is to find a partition Π , that **minimizes** the **mean** square error (MSE) computed using a test sample S^{test} and an estimation sample S^{est} , as follows:







Honest target

The goal is to find a partition Π , that **minimizes** the **mean** square error (MSE) computed using a test sample S^{test} and an estimation sample S^{est} , as follows:

$$MSE(S^{test}, S^{est}, \Pi) = \frac{1}{\#(S^{test})} \sum_{i \in S^{test}} ((Y_i - \hat{\mu}(x, S^{est}, \Pi)) - Y_i^2)$$







Honest target

The goal is to find a partition Π , that **minimizes** the **mean** square error (MSE) computed using a test sample S^{test} and an estimation sample S^{est} , as follows:

$$MSE(S^{test}, S^{est}, \Pi) = \frac{1}{\#(S^{test})} \sum_{i \in S^{test}} ((Y_i - \hat{\mu}(x, S^{est}, \Pi)) - Y_i^2)$$

In the same way, the authors also define "honest" splitting and cross-valdation.







This approach was compared to 3 other approaches (transformed outcome trees, fit-based trees, square T-statistic trees)







- This approach was compared to 3 other approaches (transformed outcome trees, fit-based trees, square T-statistic trees)
- Honest versus adaptative estimation







- This approach was compared to 3 other approaches (transformed outcome trees, fit-based trees, square T-statistic trees)
- Honest versus adaptative estimation
- New method for constructing trees for causal effects







- This approach was compared to 3 other approaches (transformed outcome trees, fit-based trees, square T-statistic trees)
- Honest versus adaptative estimation
- New method for constructing trees for causal effects
- Obtain a set of treatment effects and confidence intervals in each region







- This approach was compared to 3 other approaches (transformed outcome trees, fit-based trees, square T-statistic trees)
- Honest versus adaptative estimation
- New method for constructing trees for causal effects
- Obtain a set of treatment effects and confidence intervals in each region
- Can be used to explore randomized controlled trials (medical studies, field experiments)







- This approach was compared to 3 other approaches (transformed outcome trees, fit-based trees, square T-statistic trees)
- Honest versus adaptative estimation
- New method for constructing trees for causal effects
- Obtain a set of treatment effects and confidence intervals in each region
- Can be used to explore randomized controlled trials (medical studies, field experiments)
- Identify subsets of population with lower-than-average or higherthan-average treatment effects







- This approach was compared to 3 other approaches (transformed outcome trees, fit-based trees, square T-statistic trees)
- Honest versus adaptative estimation
- New method for constructing trees for causal effects
- Obtain a set of treatment effects and confidence intervals in each region
- Can be used to explore randomized controlled trials (medical studies, field experiments)
- Identify subsets of population with lower-than-average or higherthan-average treatment effects
- From trees to forests: *Generalized Random Forests*. Susan Athey, Julie Tibshirani and Stefan Wager(2018). In arxiv.







