# Statistical Computing

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# Statistical Computing: What will we do?

## Chapters

1. R in Action
2. Statistical Inference
3. Linear Models
4. Model Selection and Validation
5. Trees
6. Neural Nets

## Remarks

- Chapters 3 to 6:
  Statistical ML in Action
- Two weeks per chapter
- Exercises at end of chapter notes

# Trees

# Outline

- Decision Trees
- Random Forests
- Gradient Boosted Trees

# Decision Trees

- Simple
- Easy to interpret
- Decision trees are like wolves:
  Weak alone, strong together
- Around since 1984
  (Breiman, Friedman)

https://images.pexels.com/photos/3732527/pexels-photo-3732527.jpeg

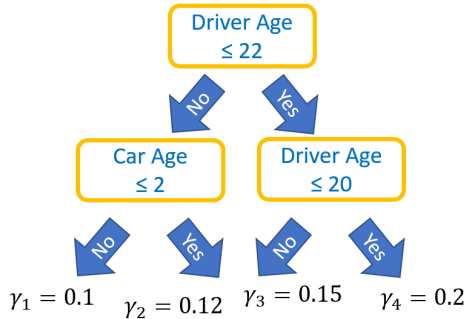
# What is a Decision Tree?

## Greedy recursive partitioning

1. Split: find best "yes/no" question on best feature to make total loss smaller
2. Apply Step 1 recursively

## Predictions

- Follow splits and use leaf value $\gamma_j$
- Usually, $\gamma_j$ is average response in leaf $j$
- Terminal regions $R_1, \ldots, R_J$
- $\boldsymbol{x}$ falls in leaf $j \Leftrightarrow \boldsymbol{x} \in R_j$
- $\hat{f}(\boldsymbol{x}) = \sum_{j=1}^{J} \gamma_j \mathbf{1}\{\boldsymbol{x} \in R_j\}$




The tree does a headstand

Example

# Properties of Decision Trees

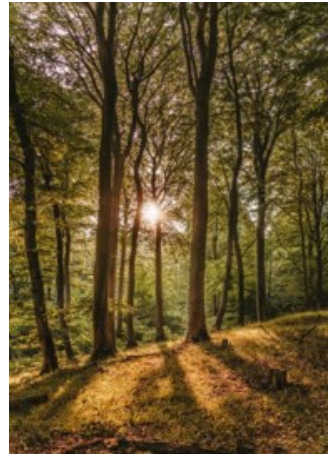
- Outliers
- Missing values
- Categorical covariates
- Greedy
- Interactions
- Extrapolation
- Instability

Most properties are inherited to groups/ensembles of decision trees

From nearest neighbors to decision trees: Short video by Jerome Friedman:
`https://www.youtube.com/watch?v=8hupHmBVvb0`

# Random Forests

- Combine many decision trees
- Perform very well
- Black Box
- Around since 2001 (Breiman)
- Why is combination of trees better than a single one?



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# Ensembling and Bagging

## Ensembling

- Combine multiple models (base learners) to single one
- Example: $k$-nearest-neighbor with different $k$
- Combined predictions have lower variance $\rightarrow$ better test performance (diversified stock portfolio, Bias-Variance Trade-Off)

## Algorithm: Bagging (Bootstrap aggregating)

1. Select $B$ bootstrapped training data sets from the original training data
2. Fit models $\hat{f}^{*j}(\boldsymbol{x})$ on them
3. Return the bagged model $\hat{f}(\boldsymbol{x}) = \frac{1}{B}\sum_{j=1}^{B}\hat{f}^{*j}(\boldsymbol{x})$

## Example

# Bias-Variance Trade-Off

Decomposition of generalization error:

$$\underbrace{\mathbb{E}(y_o - \hat{f}(x_o))^2}_{\text{Expected test MSE of } x_o} = \text{Var}(\hat{f}(x_o)) + \left[\text{Bias}(\hat{f}(x_o))\right]^2 + \underbrace{\text{Var}(\varepsilon)}_{\text{Irreducible error}}$$

(Introduction to Statistical Learning)

- One specific observation $(y_o, x_o)$
- Expectations and variances over large number of training sets
- Bias: Error introduced by approximating true model by $f$
- Low bias $\leftrightarrow$ high variance $\rightarrow$ Bias-Variance Trade-Off
- Bagged decision trees: low bias (why?) and low variance

# Remarks on Bagging

- Works best with unstable base learners $\rightarrow$ deep decision trees
- Out-of-bag (OOB) validation
- Parallel computing
- Performance versus complexity

# From Bagging to Random Forests

A random forest is a bagged decision tree with an extra twist

## Twist

- Additional source of randomness
- Each split considers only random feature subset (often $p/3$ or $\sqrt{p}$)
- Additional decorrelation $\rightarrow$ stronger diversification

## Algorithm: Random forest (regression)

1. Select $B$ bootstrapped training data sets from the original training data
2. Fit (usually deep) decision trees $\hat{f}^{*j}(\boldsymbol{x})$ on these. For each split, consider only random feature subset
3. Return the random forest $\hat{f}(\boldsymbol{x}) = \frac{1}{B} \sum_{j=1}^{B} \hat{f}^{*j}(\boldsymbol{x})$

# Comments on Random Forests

- Number of trees
- Deep trees
- Don't trust performance on training set $\rightarrow$ OOB performance
- Parameter tuning

Regarding parameter tuning: Short video by Adele Cutler on working with Leo Breiman: `https://www.youtube.com/watch?v=t8ooi_tJHSE`

Example

# Interpreting a Black Box

## Study

1. Performance
2. Variable importance
3. Effects

## XAI

- e**X**plainable **A**rtificial **I**ntelligence
- Collection of methods to interpret models
- Examples: Split-gain importance, ICE, PDP

## Example

- Split gain importance of random forest
- Variable importance and linear regression?

# Individual Conditional Expectation (ICE)

## Basic thinking

- In additive linear model $f$, the effect of $X^{(j)}$ is fully described by its coefficient(s)
- It describes how $f$ reacts on changes in $X^{(j)}$ (Ceteris Paribus)
- What if model involves complex interactions?

## Idea (Goldstein et al., 2015)

- Study (Ceteris Paribus) effect of $X^{(j)}$ for one observation
- *ICE function* for feature $X^{(j)}$ of model $f$ and observation $\boldsymbol{x} \in \mathbb{R}^p$

$$\text{ICE}_j : v \in \mathbb{R} \mapsto f(v, \boldsymbol{x}_{\setminus j})$$

- $\boldsymbol{x}_{\setminus j}$ denotes all but the $j$-th component of $\boldsymbol{x}$, which is replaced by $v$
- *ICE curve* represents graph $(v, \text{ICE}_j(v))$ for grid of values $v \in \mathbb{R}$

# ICE Plot: Visualize ICE Curves of many Observations

Example

## Notes

- Curves with different shapes indicate interaction effects
- Parallel curves $\Leftrightarrow$ additivity in $X^{(j)}$
- Centered ICE plots
- Usually on link scale (why?)

## Pros and Cons

+ Simple to compute
+ Easy to interpret (Ceteris Paribus)
+ Gives impression about interactions
– Ceteris Paribus can be unnatural
– Model applied to rare/impossible $\boldsymbol{x}$

# Partial Dependence Plot PDP (Friedman 2001)

- Average of many ICE curves
- Ceteris Paribus effect of $X^{(j)}$ averaged over all interaction effects
- (Empirical) partial dependence function of $j$-th feature

$$\text{PD}_j(v) = \frac{1}{n} \sum_{i=1}^{n} \hat{f}(v, \boldsymbol{x}_{i,\setminus j})$$

- $\boldsymbol{x}_{i,\setminus j}$ feature vector of $i$-th observation without $j$-th component
- PDP equals graph $(v, \text{PD}_j(v))$ for grid of values $v \in \mathbb{R}$
- Sum runs over reference data (=?)
- Pros/cons similar to ICE, but no info on interaction

Example

# Gradient Boosted Trees

- Combine many decision trees
- Perform very well
- Black Box
- Around since 2001 (Friedman)

} Like random forests


https://www.gormanalysis.com/blog/gradient-boosting-explained/

# Boosting

## Basic idea of boosting (e.g. Schapire, 1990)

1. Fit simple model $\hat{f}$ to data
2. For $k = 1, \ldots, K$ do:
   a. Find simple model $\hat{f}^k$ that corrects the mistakes of $\hat{f}$
   b. Update: $\hat{f} \leftarrow \hat{f} + \hat{f}^k$

## How to find updates $\hat{f}^k$?

Use decision trees $\rightarrow$ boosted trees

- Use reweighting heuristic for binary classification
  $\rightarrow$ AdaBoost (Freund and Schapire, 1995)
- Reduce total loss $Q(\hat{f} + \hat{f}^k) = \sum_{i=1}^{n} L(y_i, \hat{f}(\boldsymbol{x}_i) + \hat{f}^k(\boldsymbol{x}_i))$
  $\rightarrow$ Gradient boosting (Friedman, 2001)

# Gradient Descent

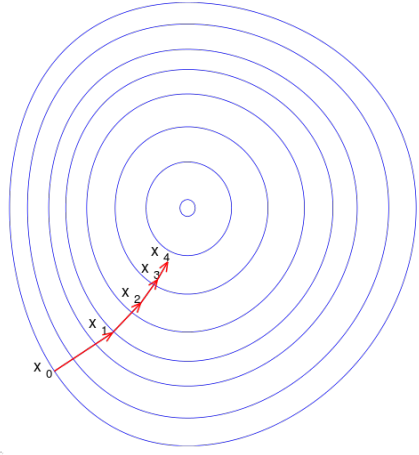
Minimize function $h : \mathbb{R}^n \to \mathbb{R}$

1. Start at some value $\hat{x} \in \mathbb{R}^n$
2. Repeat: $\hat{x} \leftarrow \hat{x} - \lambda g$

- $\lambda > 0$: Step size or learning rate
- Gradient $g \in \mathbb{R}^n$ of $h$ at $\hat{x}$:

$$g = \left[\frac{\partial h(x)}{\partial x}\right]_{x=\hat{x}}$$

- $g$ points in direction of steepest ascent




https://en.wikipedia.org/wiki/Gradient_descent

# Gradient Boosting

## Gradient descent of $Q(f)$

- $Q(f) = \sum_{i=1}^{n} L(y_i, f(\boldsymbol{x}_i))$
- $f = (f(\boldsymbol{x}_1), \ldots, f(\boldsymbol{x}_n)) \in \mathbb{R}^n$

1. Start at some value $\hat{f}$
2. Repeat: $\hat{f} \leftarrow \hat{f} - \lambda g$ with

$$g = \left[\frac{\partial Q(f)}{\partial f}\right]_{f=\hat{f}}$$

having components

$$g_i = \left[\frac{\partial L(y_i, f(\boldsymbol{x}_i))}{\partial f(\boldsymbol{x}_i)}\right]_{f(\boldsymbol{x}_i)=\hat{f}(\boldsymbol{x}_i)}$$

## For squared error?

- $L(y, z) = (y - z)^2/2$
- Plugging in: $g_i = -\underbrace{(y_i - \hat{f}(\boldsymbol{x}_i))}_{\text{Residual } r_i}$
- Repeat: $\hat{f}(\boldsymbol{x}_i) \leftarrow \hat{f}(\boldsymbol{x}_i) + \underbrace{\lambda r_i}_{\hat{f}^k?}$

## Boosting with $\hat{f}^k = -\lambda g_i$? Now way...

1. $y_i$ unknown in application
2. Should work for all $\boldsymbol{x}$

$\rightarrow$ replace $-g_i$ by predictions of tree

# Gradient Boosted Trees for Squared Error Loss

## Algorithm

1. Initialize $\hat{f}(\boldsymbol{x}) = \frac{1}{n}\sum_{i=1}^{n} y_i$
2. For $k = 1, \ldots, K$ do:
   a. For $i = 1, \ldots, n$, calculate residuals $r_i = y_i - \hat{f}(\boldsymbol{x}_i)$
   b. Model the $r_i$ as a function of the $\boldsymbol{x}_i$ by fitting a regression tree $\hat{f}^k$
   c. Update: $\hat{f}(\boldsymbol{x}) \leftarrow \hat{f}(\boldsymbol{x}) + \lambda \hat{f}^k(\boldsymbol{x})$
3. Output $\hat{f}(\boldsymbol{x})$

## General loss functions?

- Replace residuals by negative gradients of loss function
- Leaf values might be suboptimal $\rightarrow$ replace by optimal values

# Gradient Boosted Trees for General Losses

1. Initialize $\hat{f}(\boldsymbol{x}) = \text{argmin}_\gamma \sum_{i=1}^{n} L(y_i, \gamma)$
2. For $k = 1, \ldots, K$ do:
   a. For $i = 1, \ldots, n$, calculate negative gradients (pseudo-residuals)

$$r_i = -\left[\frac{\partial L(y_i, f(\boldsymbol{x}_i))}{\partial f(\boldsymbol{x}_i)}\right]_{f(\boldsymbol{x}_i)=\hat{f}(\boldsymbol{x}_i)}$$

   b. Model $r_i$ as function of $\boldsymbol{x}_i$ by regression tree $\hat{f}^k$ with terminal regions $R_1, \ldots, R_J$
   c. For each $j = 1, \ldots, J$, use line-search to find the optimal leaf value

$$\gamma_j = \text{argmin}_\gamma \sum_{\boldsymbol{x}_i \in R_j} L(y_i, \hat{f}(\boldsymbol{x}_i) + \gamma)$$

   d. Update: $\hat{f}(\boldsymbol{x}) \leftarrow \hat{f}(\boldsymbol{x}) + \lambda \underbrace{\sum_{j=1}^{J} \gamma_j \mathbf{1}\{\boldsymbol{x} \in R_j\}}_{\text{modified tree}}$

3. Output $\hat{f}(\boldsymbol{x})$

# Remarks

- Predictions are sum of short decision trees (with modified leaf values)
- Random forest: average of deep trees
- How to select learning rate $\lambda$, number of trees $K$, ...?
- (AdaBoost is gradient tree boosting with exponential loss)

# Modern Implementations

## Timeline

1. XGBoost (2014)
2. LightGBM (2016)
3. CatBoost (2017)

## Differences to Friedman's original

- Use of second order gradients
  $\rightarrow$ no line-search necessary
- Histogram binning
  $\rightarrow$ speeds up tree growth
- Penalized objective function

## Example

# Parameter Tuning is Essential

1. Number of boosting rounds/trees $K$
   $\rightarrow$ find by early stopping (validation/CV)
2. Learning rate $\lambda$
   $\rightarrow$ to get reasonable number of rounds
3. Regularization
   - Tree depth, number of leaves, loss penalties, etc.
   - $\rightarrow$ Grid/Randomized search and iterate process

## Example

- XGBoost
- LightGBM

## Comments

- Why not one big grid search on all parameters?
- Objective/metrics