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

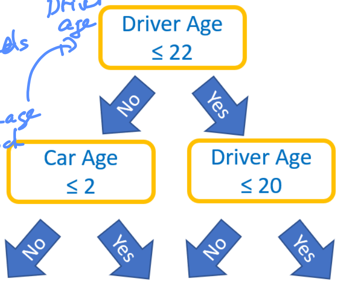
1. Split: find best “yes/no” question on best feature to make total loss smaller
2. Apply Step 1 recursively

Predictions

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

leave node value

Driver age depends on car age effect



$\gamma_1 = 0.1$ $\gamma_2 = 0.12$ $\gamma_3 = 0.15$ $\gamma_4 = 0.2$

average response

The tree does a headstand

Example

Properties of Decision Trees

outliers in response matters!

DT → interaction detection machines

- Outliers no problems normaly
  only the orders matter
- Missing values → depends on implementation
  take avg or code it (-1)
- Categorical covariates
  unordered → every subset searching
  computational expensive
- Greedy
  think just 1 step ahead

- Interactions yes, there are.
- Extrapolation outside covariate range is not possible
  → same answer for 10y old cars and 20y old cars
- Instability
  ↳ every split impacts the leave split

Most properties are inherited to groups/ensembles of decision trees

forest

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?

https://images.pexels.com/photos/1459534/pexels-photo-1459534.jpeg

Ensembling and Bagging

performance : multiple models
avg
practice : one model

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)

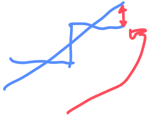
Algorithm: Bagging (Bootstrap aggregating)

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

1. Bootstrap training data
2. fit model on each
3. Avg result.

Example

Bias-Variance Trade-Off



Decomposition of generalization error:

like infinit data

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

know conceptually

Variation by taking different training sets

cannot be improved, there is no model which is better than that

- 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 → deep decision trees
- Out-of-bag (OOB) validation → 1. obs x_0 100 bagged trees: ≈ 30 are not in the bag "free cross validation"
- Parallel computing +
- Performance versus complexity
  20 models are not interpretable

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 tree $\hat{f}^{*j}(\boldsymbol{x})$ on each of them. For each split, consider only random feature subset
3. Return the random forest $\hat{f}(\boldsymbol{x}) = \frac{1}{B}\sum_{j=1}^{B} f^{*j}(\boldsymbol{x})$

Comments on Random Forests

- Number of trees
- Deep trees low bias models!
- Don't trust performance on training set $\rightarrow$ OOB performance
- Parameter tuning
  defaults usually good

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

one very important to check

Study

1. Performance
2. Variable importance
3. Effects

are those important which i thought

XAI

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

study variable importance in tree based models

how much did model gain in MSE per split

plots → applies to all models

about effects

Example

/count

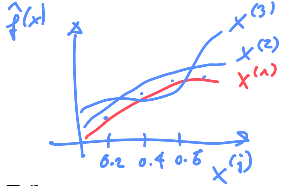
- Split gain importance of random forest
- Variable importance and linear regression?

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?

multiple numeric values



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 $\boldsymbol{x} \in \mathbb{R}^p$

interested in shape
can be different
due to interactions

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

replace x_j with v

- $\boldsymbol{x}_{\setminus j}$ denotes all but the j-th component of $\boldsymbol{x}$, which is replaced by v
- *ICE curve* represents graph $(v, \mathrm{ICE}_j(v))$ 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

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

- $\boldsymbol{x}_{i,\setminus j}$ feature vector of i-th observation without j-th component
- PDP equals graph $(v, \mathrm{PD}_j(v))$ 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

Regression case
train small tree on data
→ get residuals
train another tree on the residuals
→ iterate.

- 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: $\hat{f} \leftarrow \hat{f} + \hat{f}^k$

base learner

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

Use decision trees $\rightarrow$ boosted trees

- Use reweighting heuristic for binary classification

not well known $\rightarrow$ AdaBoost (Freund and Schapire, 1995) (check which variables has the biggest residual. $\rightarrow$ change weights)

- 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)

L typically square loss

take base learner which minimise Q
minimise a function of a function

Gradient Descent

not function space

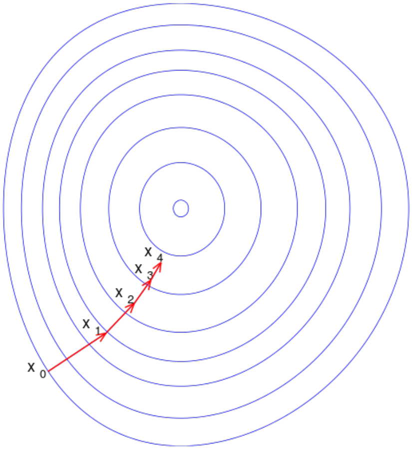
Minimize function $h : \mathbb{R}^n \to \mathbb{R}$

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 $Q(f)$

evaluating f at all training data $\in \mathbb{R}^n$

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

vector of predictions

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?

$g_i = -r_i$

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

no! can't use the response

Boosting with $\hat{f}^k = -\lambda g_i$? No~~w~~ way...

1. y_i unknown in application cannot evaluate the r_i
   prediction
2. Should work for all $\boldsymbol{x}$

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

Gradient Boosted Trees for Squared Error Loss

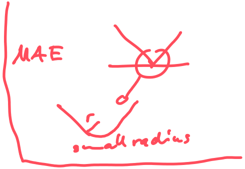
Algorithm

1. Initialize $\hat{f}(\boldsymbol{x}) = \frac{1}{n}\sum_{i=1}^{n} y_i$ save boosting rounds
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 $\hat{f}^k$
   just any model
   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 $\hat{f}(\boldsymbol{x}) = \text{argmin}_\gamma \sum_{i=1}^{n} L(y_i, \gamma)$ best constant model
2. For $k = 1, \dots, K$ do:
   a. For $i = 1, \dots, n$, calculate negative gradients (pseudo-residuals)

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

derive this once for every loss fct.

const. in terminal region

would fall in the leaf 1

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

expensive

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

Line search
what value should γ get to be optimal

   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

shrinked

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

Modern Implementations

Timeline

1. XGBoost (2014)
2. LightGBM (2016) Msft dev
3. CatBoost (2017) good on gpu by yandex

not easy to interpret

Differences to Friedman's original

- Use of second order gradients
  $\rightarrow$ no line-search necessary → newton steps
- Histogram binning caching
  $\rightarrow$ speeds up tree growth
- Penalized objective function
  # leaf nodes, L_2 penalty etc.

Example

Parameter Tuning is Essential

1. Number of boosting rounds/trees K
   $\rightarrow$ find by early stopping (validation/CV)
2. Learning rate λ $\lambda \cdot k \approx \text{const.}$
   $\lambda \cdot 10 \longrightarrow \lambda = 0.05 \longrightarrow k = 200$
   $\rightarrow$ 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? b/c λ and K are linked
  $\rightarrow$ small prob. to get good results
- Objective/metrics

0. Step.
   $\rightarrow$ choose loss function

perhaps more robust
$\hookrightarrow$ MAE $\longrightarrow$ squared error, but minimize MAE in crossvalidation