

Gradient Boosting

Evgeny Burnaev

Skoltech, Moscow, Russia

- 1 Ensembles
- 2 Naive boosting for regression
- 3 Gradient boosting
- 4 Gradient boosting: Theoretical Motivation
- 5 Gradient boosting: Loss Functions
- 6 Appendix. Gradient Boosting Decision Trees

1 Ensembles

- 2 Naive boosting for regression
- 3 Gradient boosting
- 4 Gradient boosting: Theoretical Motivation
- 5 Gradient boosting: Loss Functions
- 6 Appendix. Gradient Boosting Decision Trees

- A predictor, feature $\mathbf{x} \in \mathbb{R}^d$ has distribution D
- $f(\mathbf{x})$ is a deterministic function from some concept class
- **Goal:**
 - Based on m training pairs $\{(\mathbf{x}_i, y_i = f(\mathbf{x}_i))\}_{i=1}^m$ drawn i.i.d. from D produce a classifier $\hat{f}(\mathbf{x}) \in \{0, 1\}$
 - Choose \hat{f} to have low generalization error $R(\hat{f}) = \mathbb{E}_D [1_{\hat{f}(\mathbf{x}) \neq y}]$

- For simplicity we consider a binary classification problem. Let us denote by $h_1(\mathbf{x}), \dots, h_T(\mathbf{x})$ some binary classifiers
- Typical ensembling procedure has the form
 - Simple voting:

$$H(h_1(\mathbf{x}), \dots, h_T(\mathbf{x})) = \frac{1}{T} \sum_{t=1}^T h_t(\mathbf{x}),$$

- Weighted voting:

$$H(h_1(\mathbf{x}), \dots, h_T(\mathbf{x})) = \sum_{t=1}^T \alpha_t h_t(\mathbf{x}),$$

- Mixture of experts

$$H(h_1(\mathbf{x}), \dots, h_T(\mathbf{x})) = \sum_{t=1}^T g_t(\mathbf{x}) h_t(\mathbf{x})$$

- Final decision

$$f_T(\mathbf{x}) = \text{sign}\{H(h_1(\mathbf{x}), \dots, h_T(\mathbf{x}))\}$$

1 Ensembles

2 Naive boosting for regression

3 Gradient boosting

4 Gradient boosting: Theoretical Motivation

5 Gradient boosting: Loss Functions

6 Appendix. Gradient Boosting Decision Trees

- Consider a regression problem $\frac{1}{2} \sum_{i=1}^m (h(\mathbf{x}_i) - y_i)^2 \rightarrow \min_h$
- Search for solution in the form of weak learner composition $f_T(\mathbf{x}) = \sum_{t=1}^T h_t(\mathbf{x})$ with weak learners $h_t \in \mathbb{H}$
- The **boosting approach:** add weak learners greedily
 - Start with a “trivial” weak learner $h_0(\mathbf{x}) = \frac{1}{m} \sum_{i=1}^m y_i$
 - At step T , compute the *residuals*

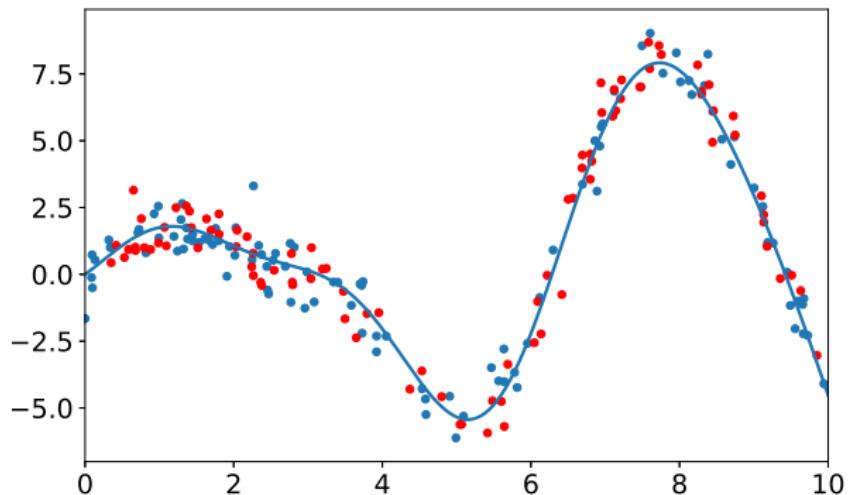
$$s_i^{(T)} = y_i - \sum_{t=1}^{T-1} h_t(\mathbf{x}_i) = y_i - f_{T-1}(\mathbf{x}_i), \quad i = 1, \dots, m$$

- Learn the next weak algorithm using

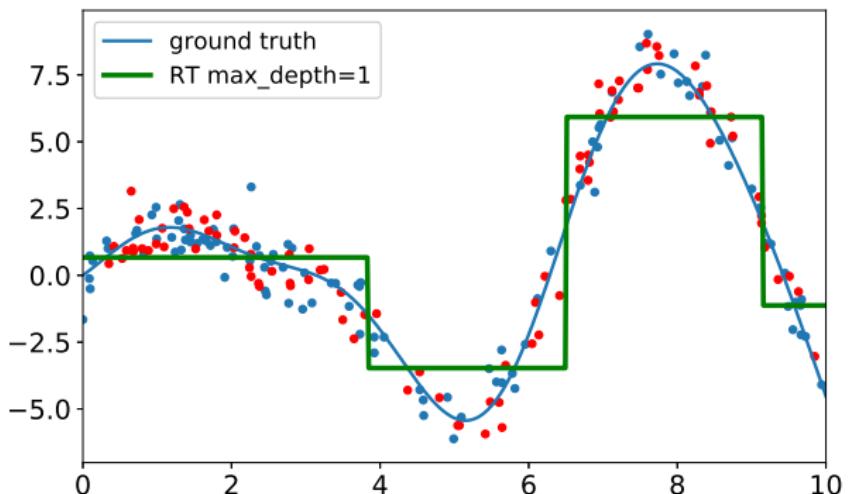
$$h_T(\mathbf{x}) := \operatorname{argmin}_{h \in \mathbb{H}} \frac{1}{2} \sum_{i=1}^m (h(\mathbf{x}_i) - s_i^{(T)})^2$$

(this implementation may be found in, e.g., scikit-learn)

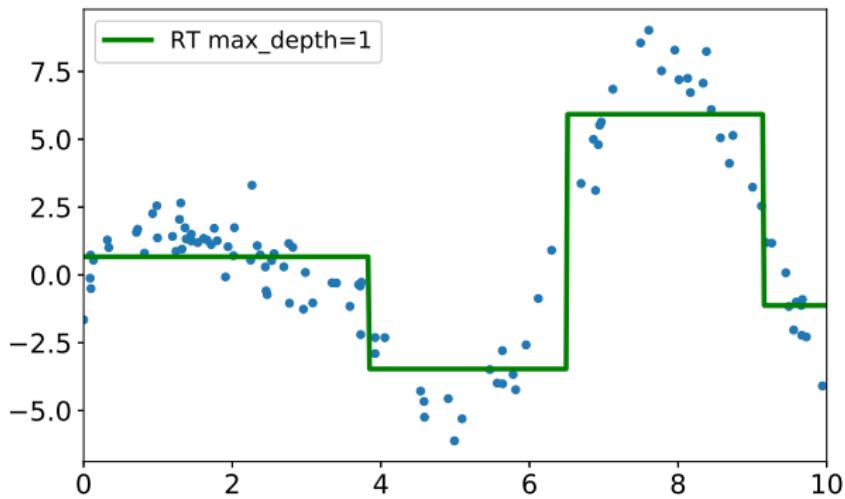
Boosting: an example regression problem



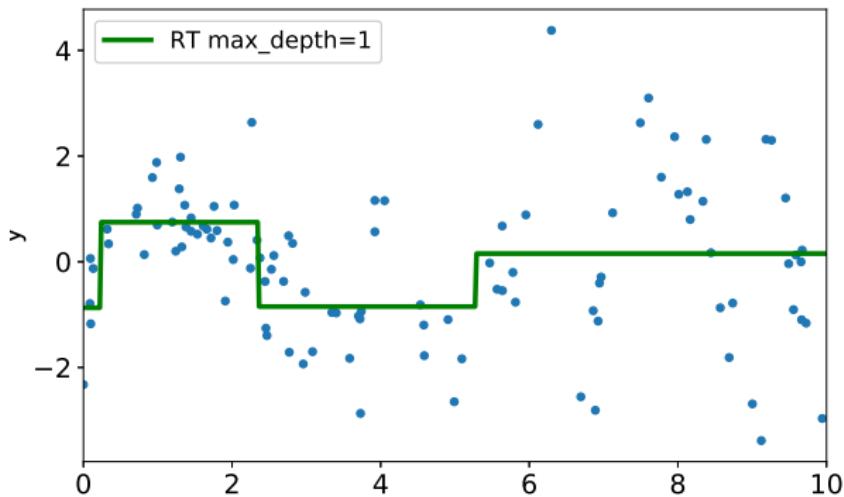
Boosting: an example regression problem



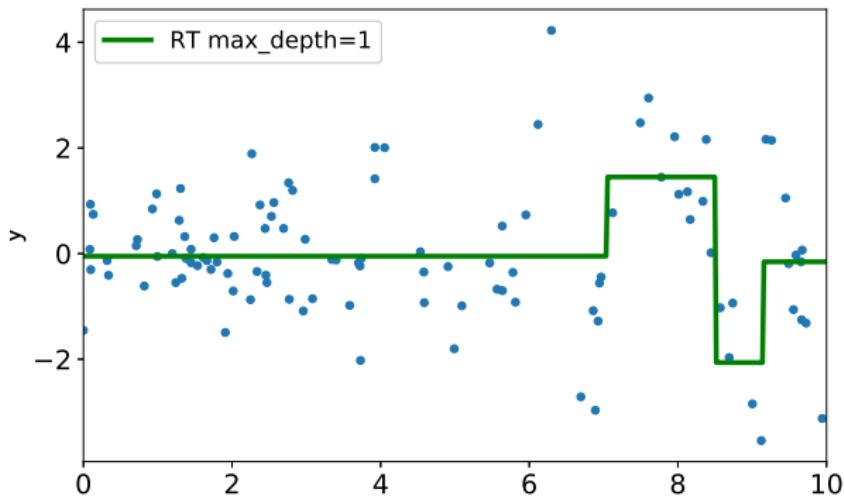
Boosting: an example regression problem



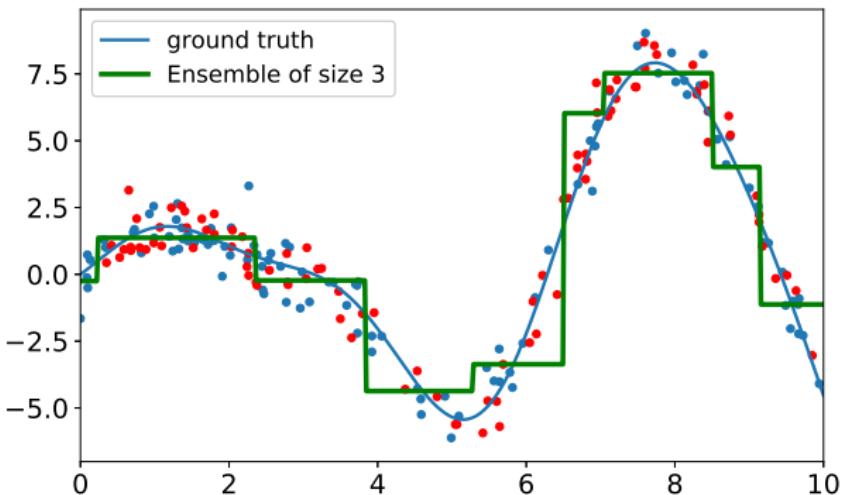
Boosting: an example regression problem



Boosting: an example regression problem



Boosting: an example regression problem



1 Ensembles

2 Naive boosting for regression

3 Gradient boosting

4 Gradient boosting: Theoretical Motivation

5 Gradient boosting: Loss Functions

6 Appendix. Gradient Boosting Decision Trees

- With $f_{T-1}(\mathbf{x})$ already built, how to find the next α_T and h_T if

$$\sum_{i=1}^m L(y_i, f_{T-1}(\mathbf{x}_i) + \alpha_T h_T(\mathbf{x}_i)) \rightarrow \min_{\alpha_T, h_T}$$

- Recall: functions decrease in the direction of negative gradient
- View $L(y, z)$ as a function of z ($= f_T(\cdot)$), execute gradient descent on z
- Search for such s_1, \dots, s_m that

$$\sum_{i=1}^m L(y_i, f_{T-1}(\mathbf{x}_i) + \alpha \cdot s_i) \rightarrow \min_{\{s_1, \dots, s_m\}, \alpha}$$

- Choose $s_i = - \left. \frac{\partial L(y_i, z)}{\partial z} \right|_{z=f_{T-1}(\mathbf{x}_i)}$
- Approximate s_i 's by $h_T(\mathbf{x})$ at $\mathbf{x} = \mathbf{x}_i$ and tune α

- Input:
 - Training set $S_m = \{(\mathbf{x}_i, y_i)\}_{i=1}^m$
 - Number of boosting iterations T
 - Loss function $L(y, z)$ with its gradient $\frac{\partial L}{\partial z}$
 - A family $\mathbb{H} = \{h(\mathbf{x})\}$ of weak learners and their associated learning procedures
 - Additional hyperparameters of weak learners (tree depth, etc.)
- Initialize GBM $h_0(\mathbf{x})$ using some simple rule (zero, most popular class, etc.)
- Execute boosting iterations $t = 1, \dots, T$ (see next slide)
- Compose the final GBM learner: $f_T(\mathbf{x}) = \sum_{t=0}^T \alpha_t h_t(\mathbf{x})$

At every iteration:

- ① Compute **pseudo-residuals**: $s_i = -\left.\frac{\partial L(y_i, z)}{\partial z}\right|_{z=f_{T-1}(\mathbf{x}_i)}, i = 1, \dots, m$
- ② Learn $h_T(\mathbf{x}_i)$ by regressing onto s_1, \dots, s_m :

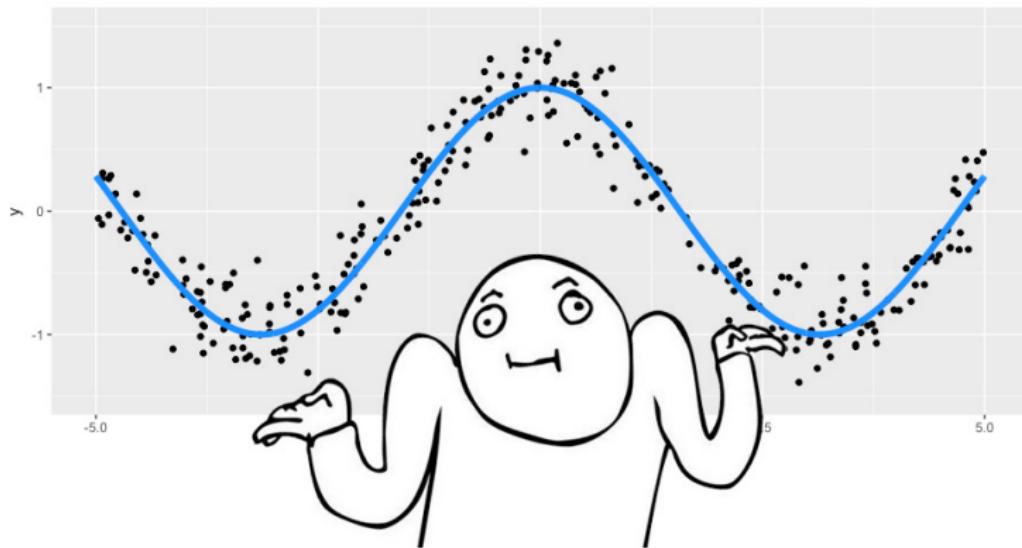
$$h_T(\mathbf{x}) = \operatorname{argmin}_{h \in \mathbb{H}} \sum_{i=1}^m (h(\mathbf{x}_i) - s_i)^2$$

- ③ Find the optimal α_N using plain gradient descent:

$$\alpha_T = \operatorname{argmin}_{\alpha \in \mathbb{R}} \sum_{i=1}^m L(y_i, f_{T-1}(\mathbf{x}_i) + \alpha h_T(\mathbf{x}_i))$$

- ④ Update the GBM by $f_T(\mathbf{x}) \leftarrow f_{T-1}(\mathbf{x}) + \alpha_T h_T(\mathbf{x})$

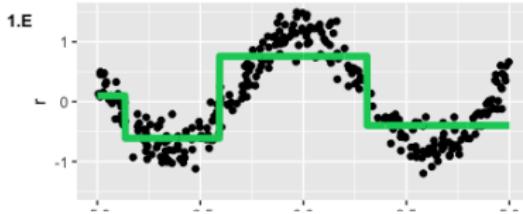
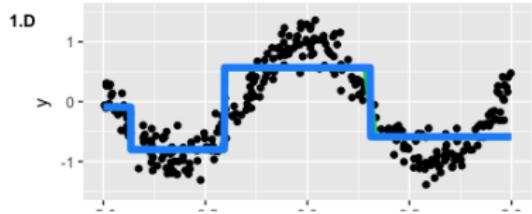
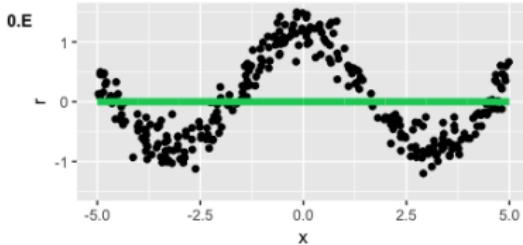
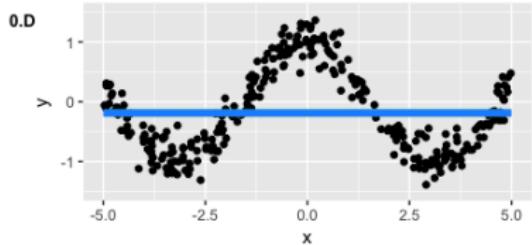
- Consider a training set for a $S_{300} = \{(\mathbf{x}_i, y_i)\}_{i=1}^{300}$ where $\mathbf{x}_i \in [-5, 5]$, $y_i = \cos(x_i) + \varepsilon_i$, $\varepsilon_i \sim \mathcal{N}(0, 1/5)$



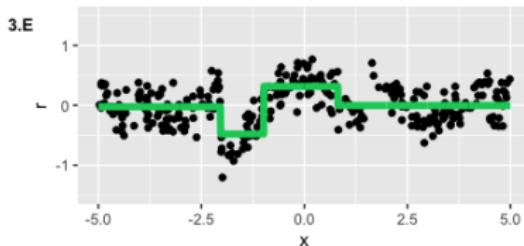
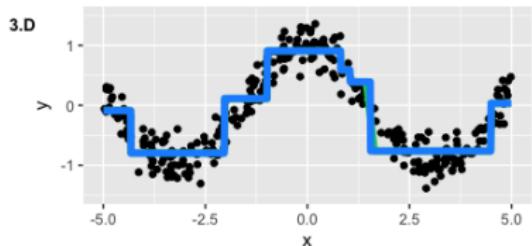
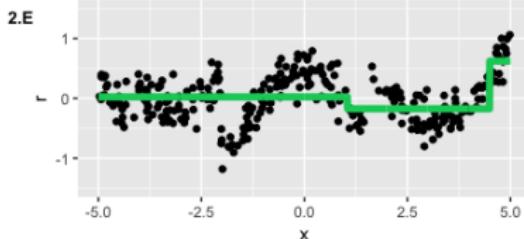
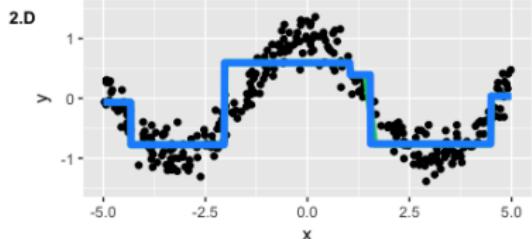
Picture credit: <https://habrahabr.ru/company/ods/blog/327250>

- Pick $T = 3$ boosting iterations
- Quadratic loss $L(y, z) = \frac{1}{2}(y - z)^2$
- Gradient of the quadratic loss $\frac{\partial L(y_i, z)}{\partial z} = -(y - z)$ is just residuals
- Pick decision trees as weak learners $h_t(\mathbf{x})$
- Set 2 as the maximum depth for decision trees

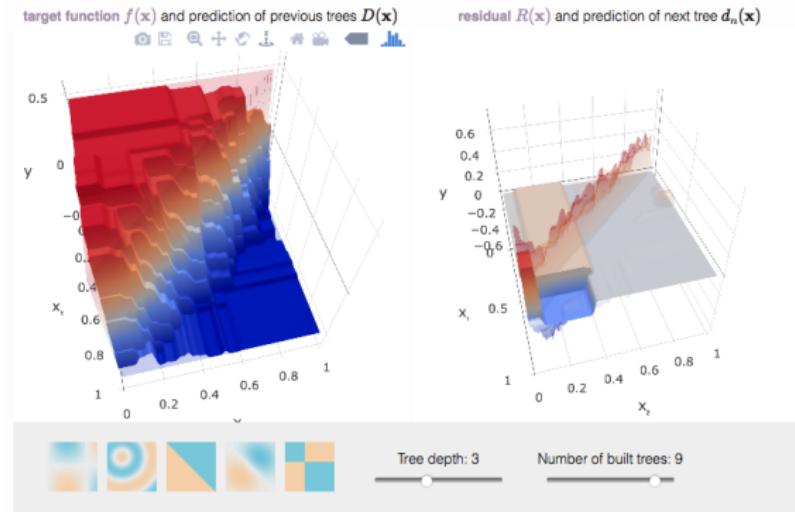
GBM: an example regression problem



GBM: an example regression problem



http://arogozhnikov.github.io/2016/06/24/gradient_boosting_explained.html

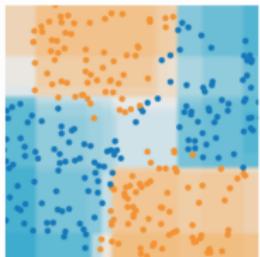


http://arogozhnikov.github.io/2016/07/05/gradient_boosting_playground.html

Dataset to classify:



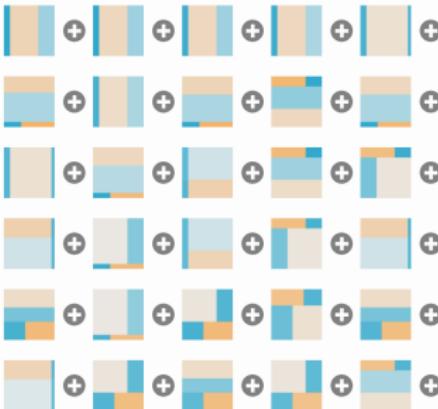
Prediction:



↑
predictions of GB (all 50 trees)

train loss: 0.266 test loss: 0.312

Decision functions of first 30 trees



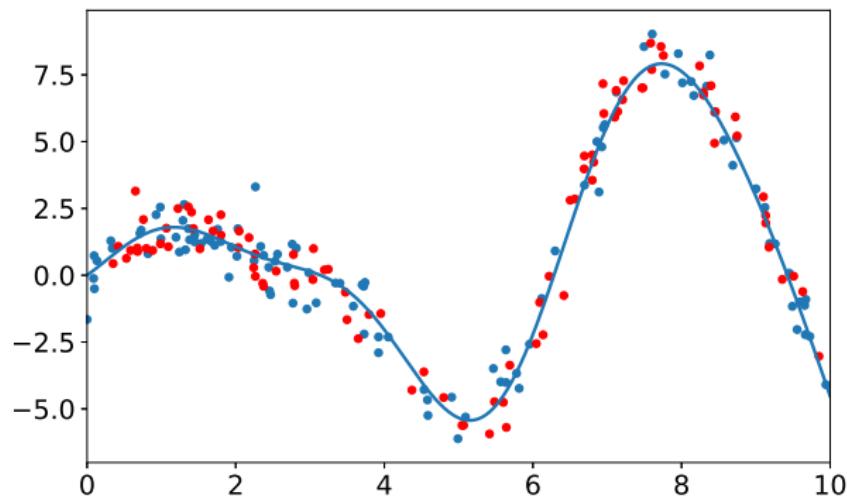
- For **too simple weak learners**, the negative gradient is approximated badly \implies random walk in space of samples
- For **too complex weak learners**, a few boosting steps may be enough for overfitting
- **Shrinkage:** make shorter steps using a *learning rate* $\eta \in (0, 1]$

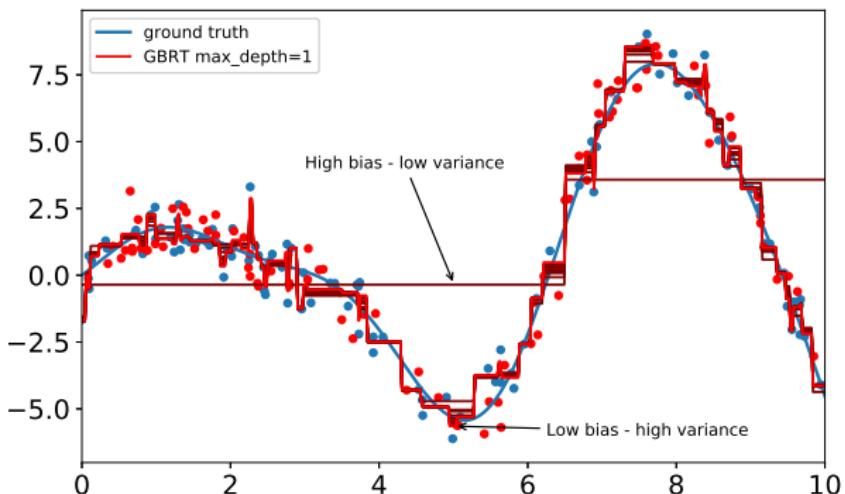
$$f_T(\mathbf{x}_i) \leftarrow f_{T-1}(\mathbf{x}) + \eta \alpha_T h_T(\mathbf{x})$$

(effectively distrust gradient direction estimated via weak learners)

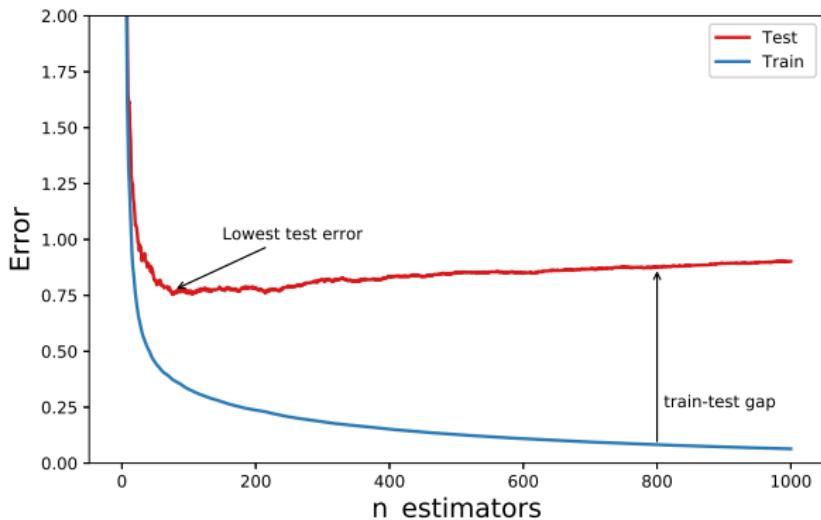
Figure – High shrinkage

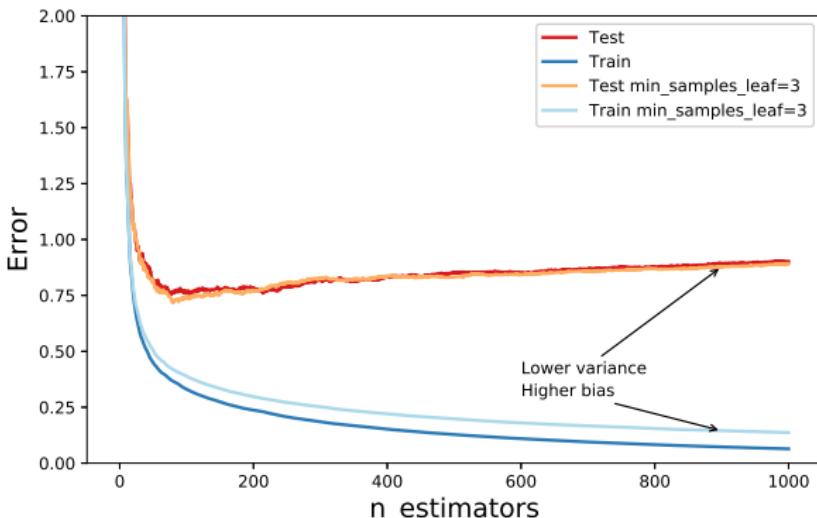
Figure – Low shrinkage

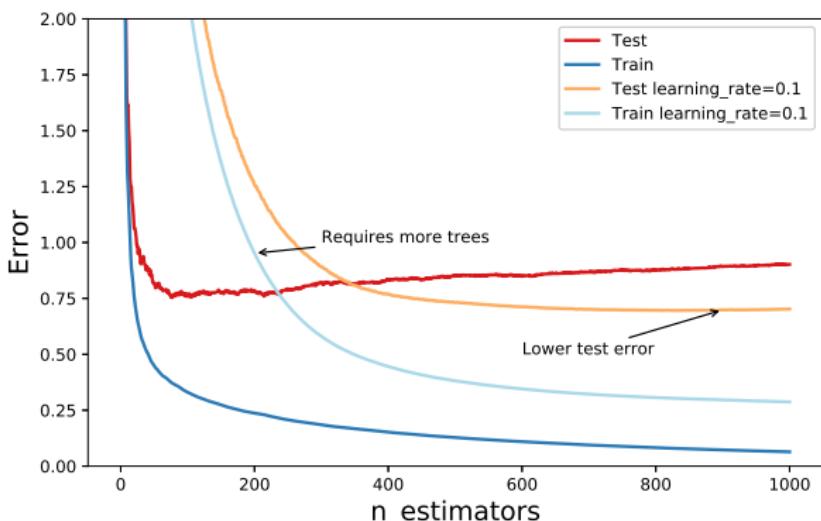


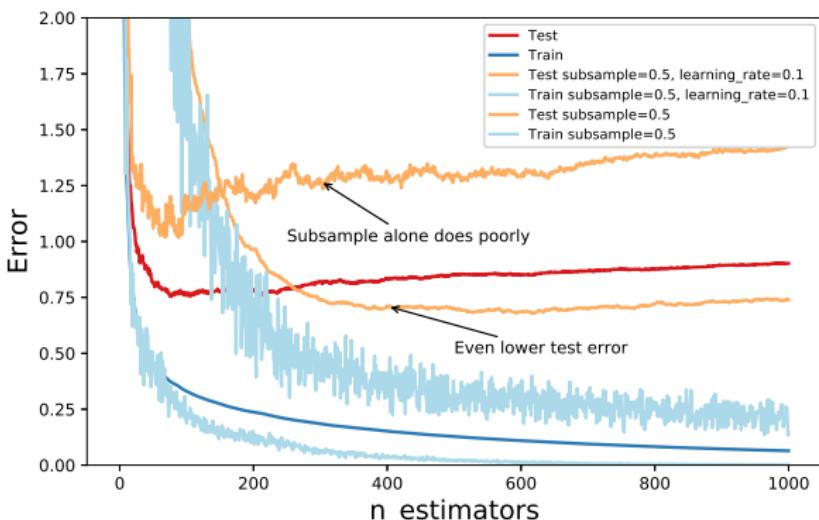


GBM: regularization approaches









1 Ensembles

2 Naive boosting for regression

3 Gradient boosting

4 Gradient boosting: Theoretical Motivation

5 Gradient boosting: Loss Functions

6 Appendix. Gradient Boosting Decision Trees

- **Output (response)**: a random variable y
- **Input (explanatory)**: a set of random variables $\mathbf{x} = (x_1, \dots, x_d)$
- Training sample $S_m = \{(\mathbf{x}_i, y_i)\}_{i=1}^m$ of $(\mathbf{x}_i, y_i) \sim D$
- Let $f^*(\mathbf{x})$ minimizes the expected loss value $L(y, f(\mathbf{x}))$

$$f^* = \arg \inf_f \mathbb{E}_D L(y, f(\mathbf{x}))$$

- **Goal**: obtain an estimate $\hat{f}(\mathbf{x})$ of the function $f^*(\mathbf{x})$

- We apply numerical optimization in function space
- We
 - consider $f(\mathbf{x})$ evaluated at each point \mathbf{x} as a parameter and
 - seek to minimize

$$\varPhi(f) = \mathbb{E}_{y, \mathbf{x}} L(y, f(\mathbf{x})) = \mathbb{E}_{\mathbf{x}} [\mathbb{E}_y L(y, f(\mathbf{x})) | \mathbf{x}]$$

at each individual \mathbf{x} , directly with respect to $f(\mathbf{x})$

- Numerical optimization: we approximate $f^*(\mathbf{x})$ by

$$f_T(\mathbf{x}) = \sum_{t=0}^T h_t(\mathbf{x}),$$

where $h_0(\mathbf{x})$ is an initial guess, and $\{h_t(\mathbf{x})\}_{t=1}^T$ are incremental functions (steps or boosts)

- Steepest-descent:

$$h_t(\mathbf{x}) = -\alpha_t g_t(\mathbf{x})$$

with

$$g_t(\mathbf{x}) = \left[\frac{\partial \Phi(f(\mathbf{x}))}{\partial f(\mathbf{x})} \right]_{f(\mathbf{x})=f_{t-1}(\mathbf{x})}$$

and

$$f_{t-1}(\mathbf{x}) = \sum_{s=0}^{t-1} h_s(\mathbf{x})$$

- The multiplier α_t is given by the line search

$$\alpha_t = \arg \min_{\alpha} \mathbb{E}_D L(y, f_{t-1}(\mathbf{x}) - \alpha g_t(\mathbf{x}))$$

Idea: let us find such model $h_T(\mathbf{x})$, such that it approximates antigradient $\{-g_T(\mathbf{x}_i)\}_{i=1}^m$

$$h_T = \arg \max_h \sum_{i=1}^m \{(-g_T(\mathbf{x}_i)) - h(\mathbf{x}_i)\}^2$$

1 Ensembles

2 Naive boosting for regression

3 Gradient boosting

4 Gradient boosting: Theoretical Motivation

5 Gradient boosting: Loss Functions

6 Appendix. Gradient Boosting Decision Trees

Loss Function: $L(y, f) = \frac{1}{2}(y - f)^2$

Algorithm:

1. $f_0(\mathbf{x}) = \frac{1}{m} \sum_{i=1}^m y_i$
2. For $t = 1$ to T do
 - $s_i = - \left[\frac{\partial L(y_i, f(\mathbf{x}_i))}{\partial f(\mathbf{x}_i)} \right]_{f(\mathbf{x})=f_{t-1}(\mathbf{x})} = y_i - f_{t-1}(\mathbf{x}_i), i \in [1, m]$
 - $(\alpha_t, \mathbf{w}_t) = \arg \min_{\mathbf{w}, \alpha} \sum_{i=1}^m [s_i - \alpha h(\mathbf{x}_i; \mathbf{w})]^2$
 - $f_t(\mathbf{x}) = f_{t-1}(\mathbf{x}) + \alpha_t h(\mathbf{x}; \mathbf{w}_t)$

- Loss Function: $L(y, F) = |y - f|$,

$$s_i = \text{sign}(y_i - f_{t-1})$$

- Consider the special case where each base learner is a J -terminal node regression tree. Each regression tree has the additive form

$$h(\mathbf{x}; \mathbf{w} = \{a_j, R_j\}_{j=1}^J) = \sum_{j=1}^J a_j \mathbf{1}(\mathbf{x} \in R_j)$$

- $\{R_j\}_{j=1}^J$ are disjoint regions that collectively cover the space of all values of the predictor variable \mathbf{x}

Algorithm:

1. $f_0(\mathbf{x}) = \text{median}\{y_i, i \in [1, m]\}$
2. For $t = 1$ to T do
 - $s_i = \text{sign}(y_i - f_{t-1}(\mathbf{x}_i)), i \in [1, m]$
 - $\{R_{j,t}\}_{j=1}^J = J - \text{terminal node tree}(\{s_i, \mathbf{x}_i\}_{i=1}^m)$
 - $w_{j,t} = \text{median}\{y_i - f_{t-1}(\mathbf{x}_i), \mathbf{x}_i \in R_{j,t}\}, j \in [1, J]$
 - $f_t(\mathbf{x}) = f_{t-1}(\mathbf{x}) + \sum_{j=1}^J w_{j,t} \mathbf{1}(\mathbf{x} \in R_{j,t})$

The LAD algorithm is highly robust:

- Trees use only order information on the individual variables x_k
- Pseudo-responses s_i have only two values, $s_i \in \{-1, +1\}$
- Terminal node updates are based on medians

- M -regression
- Two-class logistic regression and classification
- Multiclass logistic regression and classification

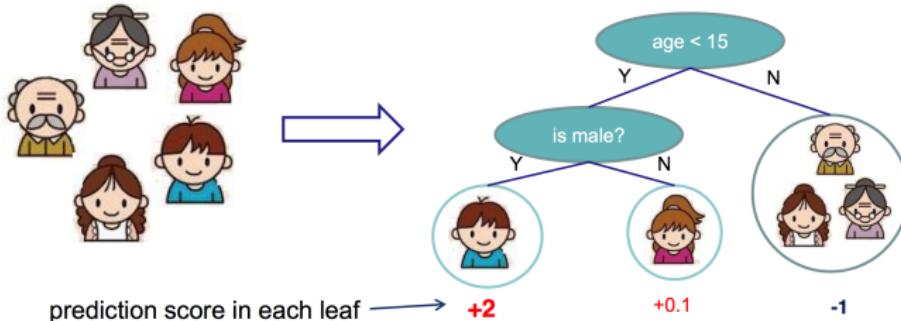
- On each of boosting steps use some randomly selection subsample
- Usually
 - accuracy is improved
 - convergence is improved
 - learning time is decreased

- 1 Ensembles
- 2 Naive boosting for regression
- 3 Gradient boosting
- 4 Gradient boosting: Theoretical Motivation
- 5 Gradient boosting: Loss Functions
- 6 Appendix. Gradient Boosting Decision Trees

- Classification and Regression Trees:

- Decision rules
- Contains one score in each leaf value

Input: age, gender, occupation,... \Rightarrow Does the person like computer games?



- Model: we have T trees

$$f_T(\mathbf{x}) = \sum_{t=1}^T h_t(\mathbf{x}), \quad h_t(\mathbf{x}) \in \mathbb{H},$$

where \mathbb{H} is a space of functions, containing all decision trees

- Parameters: structure of each tree, and the score in the leaf

- Objective: $R(\mathbf{w}) = \sum_{i=1}^m L(y_i, \hat{y}_i) + \sum_{t=1}^T \Omega(h_t)$
- We can not use methods such as SGD, to find f_T (since parameters are trees, instead of just numerical vectors) → **Additive Training (Boosting)**
 - Start from constant prediction, add a new function each time

$$\hat{y}^{(0)} = h_0(\mathbf{x}) = 0$$

$$\hat{y}^{(1)} = h_1(\mathbf{x}) = \hat{y}^{(0)} + h_1(\mathbf{x})$$

$$\hat{y}^{(2)} = h_1(\mathbf{x}) + h_2(\mathbf{x}) = \hat{y}^{(1)} + h_2(\mathbf{x})$$

...

$$\hat{y}^{(t)} = \sum_{s=1}^t h_s(\mathbf{x}) = \hat{y}^{(t-1)} + h_t(\mathbf{x})$$

- Iterative Objective Optimization
- At round t we need to tune $h_t(\mathbf{x})$

$$\begin{aligned} R^{(t)} &= \sum_{i=1}^m L\left(y_i, \hat{y}_i^{(t)}\right) + \sum_{s=1}^t \Omega(h_s) \\ &= \sum_{i=1}^m L\left(y_i, \hat{y}_i^{(t-1)} + h_t(\mathbf{x}_i)\right) + \Omega(h_t) + \text{const} \end{aligned}$$

- Consider squared loss

$$\begin{aligned} R^{(t)} &= \sum_{i=1}^m \left(y_i - \left(\hat{y}_i^{(t-1)} + h_t(\mathbf{x}_i) \right) \right)^2 + \Omega(h_t) + \text{const} \\ &= \sum_{i=1}^m \left[2 \left(\hat{y}_i^{(t-1)} - y_i \right) h_t(\mathbf{x}_i) + h_t^2(\mathbf{x}_i) \right] + \Omega(h_t) + \text{const} \end{aligned}$$

- Goal: optimize $R^{(t)} = \sum_{i=1}^m L\left(y_i, \hat{y}_i^{(t-1)} + h_t(\mathbf{x}_i)\right) + \Omega(h_t) + \text{const}$
→ computationally complicated
- Taylor expansion:

$$R^{(t)} \approx \sum_{i=1}^m \left[L\left(y_i, \hat{y}_i^{(t-1)}\right) + g_i h_t(\mathbf{x}_i) + \frac{1}{2} d_i h_t^2(\mathbf{x}_i) \right] + \Omega(h_t) + \text{const}, \text{ where}$$

$$g_i = \partial_{\hat{y}^{(t-1)}} L\left(y_i, \hat{y}^{(t-1)}\right), \quad d_i = \partial_{\hat{y}^{(t-1)}}^2 L\left(y_i, \hat{y}^{(t-1)}\right)$$

- In case of a squared loss

$$g_i = \partial_{\hat{y}^{(t-1)}} \left(\hat{y}^{(t-1)} - y_i \right)^2 = 2 \left(\hat{y}^{(t-1)} - y_i \right),$$

$$d_i = \partial_{\hat{y}^{(t-1)}}^2 \left(\hat{y}^{(t-1)} - y_i \right)^2 = 2$$

- **Objective:**

$$\sum_{i=1}^m \left[g_i h_t(\mathbf{x}_i) + \frac{1}{2} d_i h_t^2(\mathbf{x}_i) \right] + \Omega(h_t), \text{ where}$$

$$g_i = \partial_{\hat{y}^{(t-1)}} l(y_i, \hat{y}^{(t-1)}), \quad d_i = \partial_{\hat{y}^{(t-1)}}^2 l(y_i, \hat{y}^{(t-1)})$$

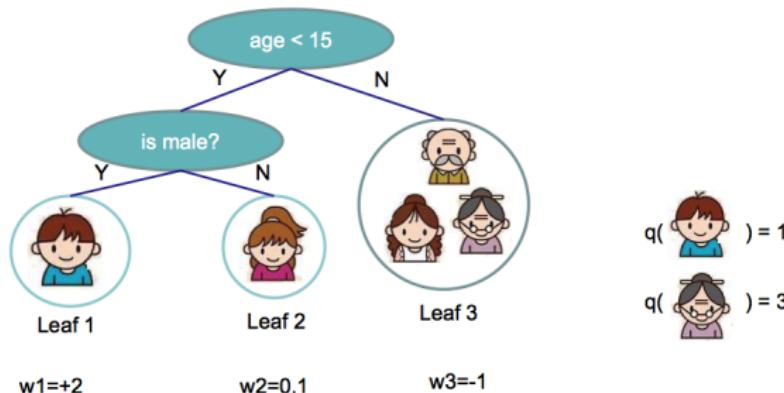
- Approximation of the objective depends on $l(\cdot, \cdot)$ only through g_i and d_i . Thus using it we can
 - Computationally efficiently control growing of trees
 - Easily introduce different loss functions $l(\cdot, \cdot)$ inside boosted trees implementation

- We define a tree by a vector of scores in leafs, and a leaf index mapping function that maps an instance to a leaf

$$h_t(\mathbf{x}) = w_{q(\mathbf{x})},$$

where

- $\mathbf{w} = (w_1, \dots, w_J) \in \mathbb{R}^J$ are the leaf weights of the tree
- $q : \mathbf{x} \rightarrow \{1, 2, \dots, J\}$ is the structure of the tree

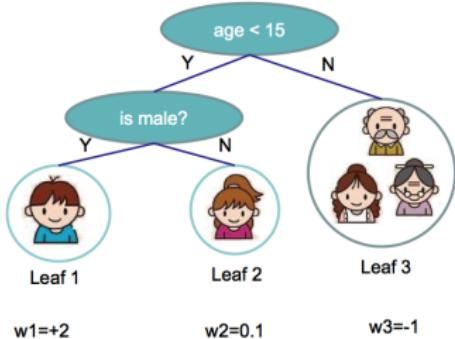


- Define complexity as (this is not the only possible definition)

$$\Omega(h_t) = \gamma J + \frac{1}{2} \lambda \sum_{j=1}^J \omega_j^2,$$

where

- J is a number of leaves in h_t
- L_2 -norm of leaf scores in h_t is used as a regularizer



$$\Omega = \gamma \cdot 3 + \frac{1}{2} \lambda (4 + 0.01 + 1)$$

- Define the instance set in the leaf j as $I_j = \{i \mid q(\mathbf{x}_i) = j\}$
- Re-group the objective by each leaf

$$\begin{aligned} R^{(t)} &\approx \sum_{i=1}^m \left[g_i h_t(\mathbf{x}_i) + \frac{1}{2} d_i h_t^2(\mathbf{x}_i) \right] + \Omega(h_t) \\ &= \sum_{i=1}^m \left[g_i w_{q(\mathbf{x}_i)} + \frac{1}{2} d_i w_{q(\mathbf{x}_i)}^2 \right] + \gamma J + \lambda \frac{1}{2} \sum_{j=1}^J w_j^2 \\ &= \sum_{j=1}^J \left[\left(\sum_{i \in I_j} g_i \right) w_j + \frac{1}{2} \left(\sum_{i \in I_j} d_i + \lambda \right) w_j^2 \right] + \gamma J \end{aligned}$$

- This is a sum of J independent quadratic functions

- Let us define $G_j = \sum_{i \in I_j} g_i$, $D_j = \sum_{i \in I_j} d_i$

$$R^{(t)} \approx \sum_{j=1}^J \left[G_j w_j + \frac{1}{2} (D_j + \lambda) w_j^2 \right] + \gamma J$$

- Assume the structure of the tree (defined by the function $q(\mathbf{x})$) is fixed, then the optimal weight in each leaf, and the resulting objective value are

$$\omega_j^* = -\frac{G_j}{D_j + \lambda}, R^{(t)} = -\frac{1}{2} \sum_{j=1}^J \frac{G_j^2}{D_j + \lambda} + \gamma J$$

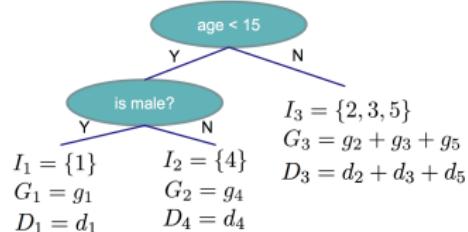


- The term (*) measure how good a tree structure is

Calculation of the Objective

Instance index gradient statistics

1		g1, d1
2		g2, d2
3		g3, d3
4		g4, d4
5		g5, d5



$$R^{(t)} = -\frac{1}{2} \sum_j \frac{G_j^2}{D_j + \lambda} + 3\gamma$$

The smaller the score is, the better the structure is

- Enumerate the possible tree structures by $q(\mathbf{x})$
- Calculate the structure score for the $q(\mathbf{x})$, using the scoring equation

$$R^{(t)} = -\frac{1}{2} \sum_{j=1}^J \frac{G_j^2}{D_j + \lambda} + \gamma J$$

- Find the best tree structure, and use the optimal leaf weight

$$w_j^* = -\frac{G_j}{D_j + \lambda}$$

- However, there can be infinite possible tree structures

In practice, we grow the tree greedily

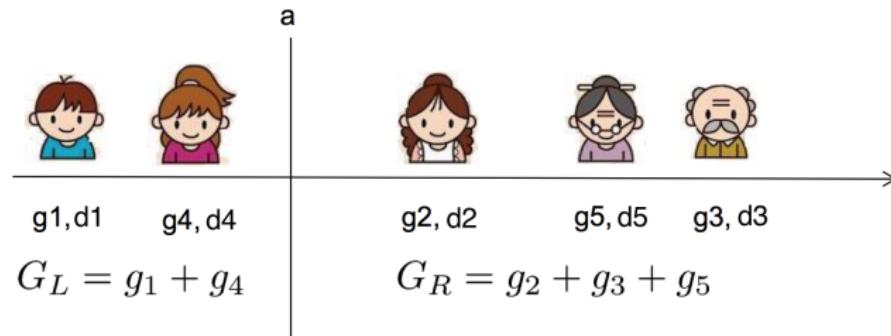
- Start from a tree with depth 0
- For each leaf node of the tree, try to add a split. The change of objective after adding the split is

$$\Delta R^{(t)} = \underbrace{\frac{G_L^2}{D_L + \lambda}}_{(1)} + \underbrace{\frac{G_R^2}{D_R + \lambda}}_{(2)} - \underbrace{\frac{(G_L + G_R)^2}{D_L + D_R + \lambda}}_{(3)} - \underbrace{\gamma}_{(4)},$$

where

- (1) and (2) are scores of Left and Right childs,
- (3) is the score if we do not split
- (4) is the complexity cost by introducing additional leaf
- How do we find the best split?

- What is the gain of a split rule $x_k < a$? E.g. x_k is an age



- We sum g 's and d 's in each leaf and calculate

$$\Delta R^{(t)} = \frac{G_L^2}{D_L + \lambda} + \frac{G_R^2}{D_R + \lambda} - \frac{(G_L + G_R)^2}{D_L + D_R + \lambda} - \gamma,$$

- Left to right linear scan over sorted instances is enough to decide the best split along the feature x_k

- The **Gradient Boosting Machine**: a general approach to boosting adding weak learners that approximate gradient of the loss function
- Gradient Boosting is the most general
 - any loss function
 - good for classification, regression, ranking
- Usually Stochastic gradient boosting is more accurate and faster
- GB is usually applied to decision trees
- In practice GB works only with big T and weak learners (small T and strong learner are not efficient)
- **AdaBoost**: gradient boosting with an exponential loss function resulting in reweighting training instances when adding weak learners
- **XGBoost**: gradient boosting with second order optimization, penalized loss and particular choice of impurity criterion