Lecture 12: 27 February, 2025

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Data Mining and Machine Learning
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Limitations of classification models

Recall

- Bias : Expressiveness of model limits classification
- Variance: Variation in model based on sample of training data

Overcoming limitations

- Bagging is an effective way to overcome high variance
  - Ensemble models
    - Sequence of models based on independent bootstrap samples
    - Use voting to get an overall classifier
- How can we cope with high bias?

Dealing with bias

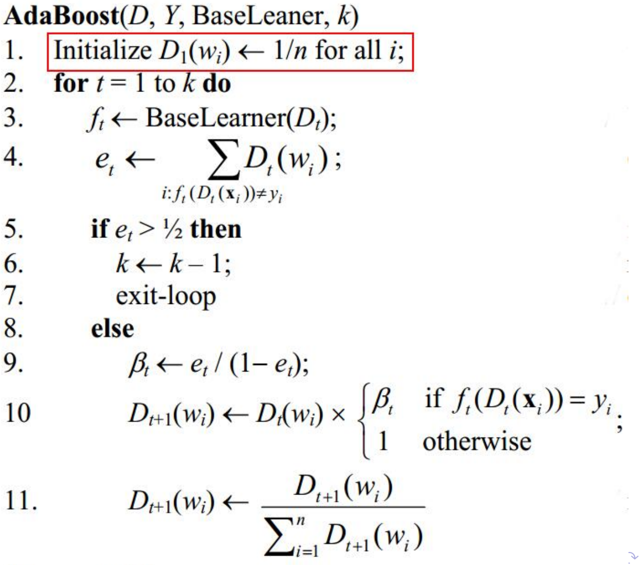
- A biased model always makes mistakes
    - Build an ensemble of models to average out mistakes
- Mistakes should be compensated across models in the ensemble
    - How to build a sequence of models, each biased a different way?
    - Again, we assume we have only one set of training data

Boosting

- Build a sequence of weak classifiers $M_1, M_2, \ldots, M_n$ on inputs $D_1, D_2, \ldots, D_n$
  - A weak classifier is any classifier that has error rate strictly below 50%
- Each D_i is a weighted variant of original training data D
  - Initially all weights equal, D_1
  - Going from D_i to D_{i+1} : increase weights where M_i makes mistakes on D_i
  - M_{i+1} will compensate for errors of M_i
- Also, each model M_i gets a weight α_i based on its accuracy on D_i
- Ensemble output
  - Individual classification outcomes are $\{-1, +1\}$
  - Unknown input x: ensemble outcome is weighted sum $\displaystyle\sum_{i=1}^{n} \alpha_i M_i(x)$
  - Check if weighted sum is negative/positive

The boosting algorithm — Adaboost

- Initially, all data items have equal weight



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    $\boxed{\text{Initialize } D_1(w_i) \leftarrow 1/n \text{ for all } i;}$
    for $t = 1$ to $k$ do
        $f_t \leftarrow$ BaseLearner($D_t$);
        $e_t \leftarrow \sum_{i: f_t(D_t(\mathbf{x}_i)) \neq y_i} D_t(w_i)$;
        if $e_t > \frac{1}{2}$ then
            $k \leftarrow k - 1$;
            exit-loop
        else
            $\beta_t \leftarrow e_t / (1 - e_t)$;
            $D_{t+1}(w_i) \leftarrow D_t(w_i) \times \begin{cases} \beta_t & \text{if } f_t(D_t(\mathbf{x}_i)) = y_i \\ 1 & \text{otherwise} \end{cases}$;
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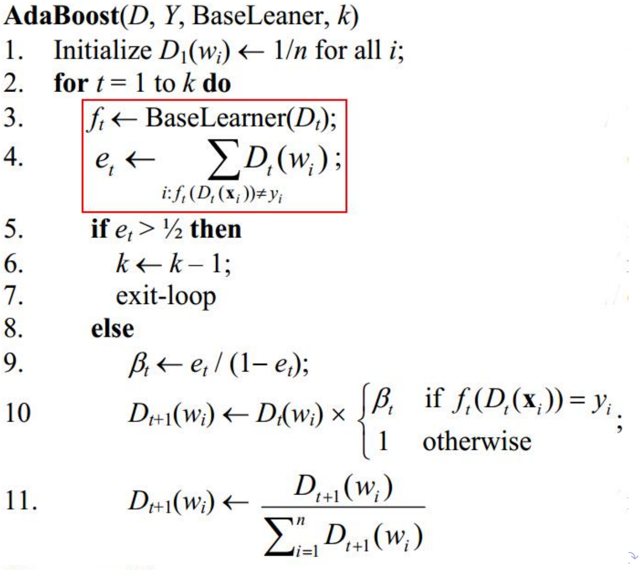
The boosting algorithm — Adaboost

- Initially, all data items have equal weight
- Build a new model and compute its weighted error



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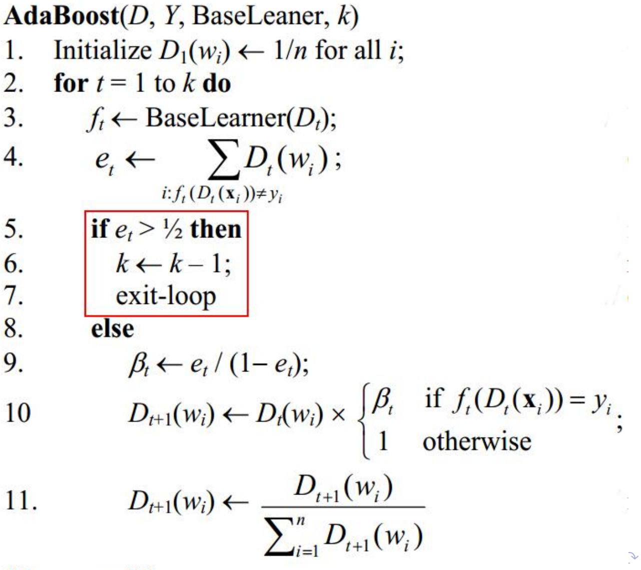
The boosting algorithm — Adaboost

- Initially, all data items have equal weight
- Build a new model and compute its weighted error
- Discard if error rate is above 50%



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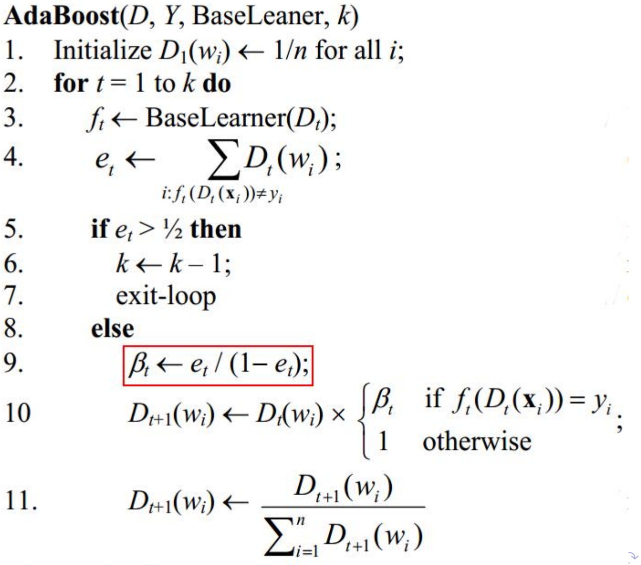
The boosting algorithm — Adaboost

- Initially, all data items have equal weight
- Build a new model and compute its weighted error
- Discard if error rate is above 50%
- Damping factor — reduce weight of correct inputs



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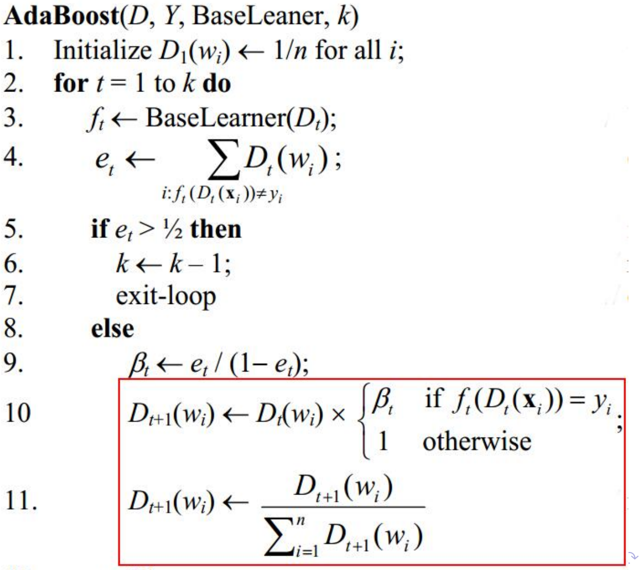
The boosting algorithm — Adaboost

- Initially, all data items have equal weight
- Build a new model and compute its weighted error
- Discard if error rate is above 50%
- Damping factor — reduce weight of correct inputs
- Reweight data items and normalize



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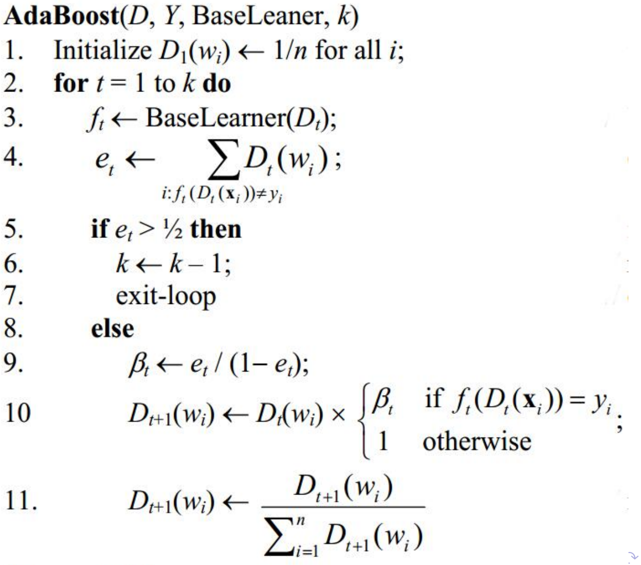
The boosting algorithm — Adaboost

- Initially, all data items have equal weight
- Build a new model and compute its weighted error
- Discard if error rate is above 50%
- Damping factor — reduce weight of correct inputs
- Reweight data items and normalize
- Final classifier

$$f_{\text{final}}(x) = \arg\max_{y \in Y} \sum_{t: f_t(x) = y} \log \frac{1}{\beta_t}$$



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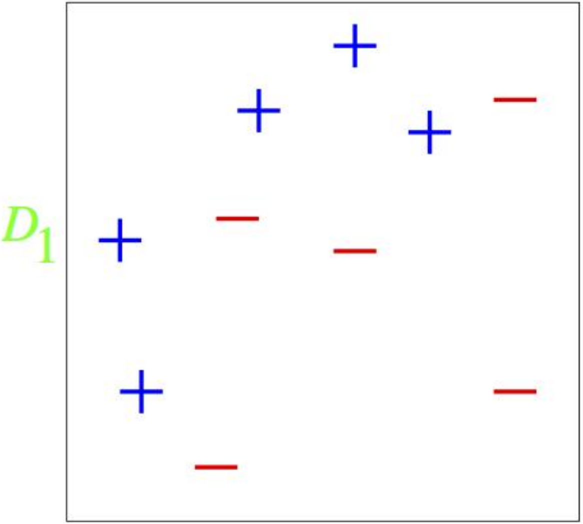
The boosting algorithm — Adaboost

- Each M_i could be a different type of model
- Start with N weak classifiers
- Initially all data items have equal weight, select M_1 as model with lowest error rate among N candidates
- Inductively, assume we have selected $M_1, \ldots M_j$, with model weights $\alpha_1, \ldots,$ α_j, and dataset is updated with new weights as D_{j+1}
  - Pick model with lowest error rate on D_{j+1} as M_{j+1}
  - Calculate α_{j+1} based on error rate of M_{j+1}
  - Reweight all training data based on error rate of M_{j+1}
- Note that same model M may be picked in multiple iterations, assigned different weights α

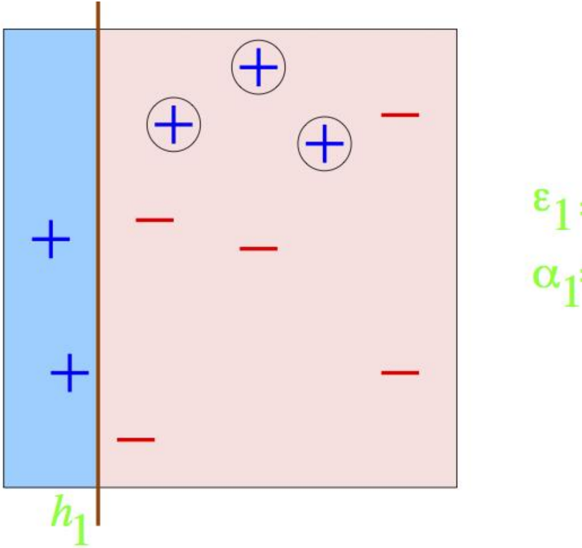
Boosting: An example

- Weak classifiers are horizontal and vertical lines
- Initial training data has equal weights



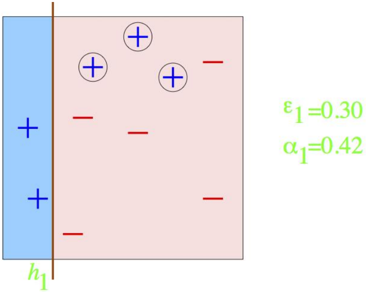
Boosting: An example

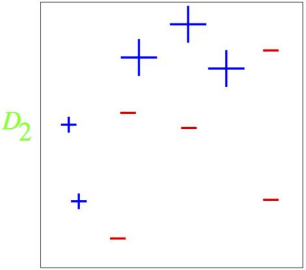
- Weak classifiers are horizontal and vertical lines
- Initial training data has equal weights
- First separator: vertical line



Boosting: An example

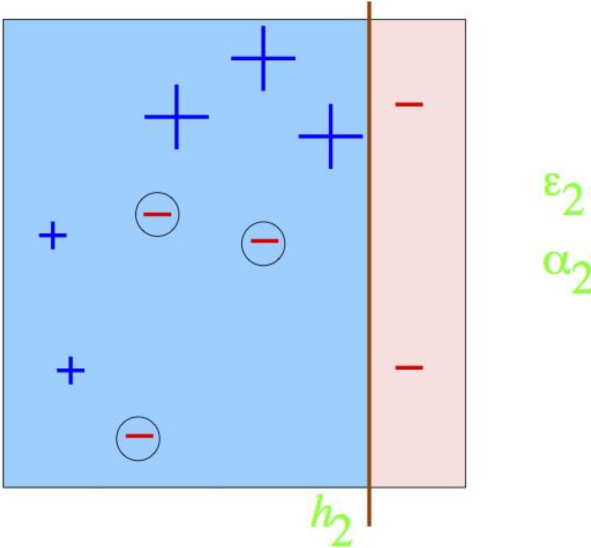
- Weak classifiers are horizontal and vertical lines
- Initial training data has equal weights
- First separator: vertical line
  - Increase weight of misclassified inputs





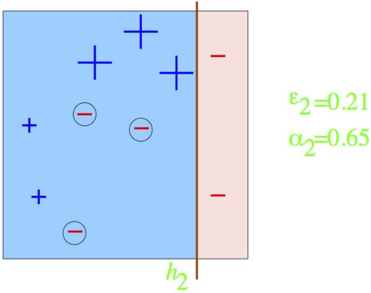
Boosting: An example

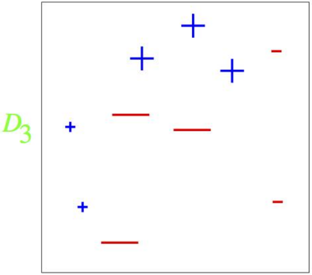
- Weak classifiers are horizontal and vertical lines
- Initial training data has equal weights
- First separator: vertical line
  - Increase weight of misclassified inputs
- Second separator: vertical line



Boosting: An example

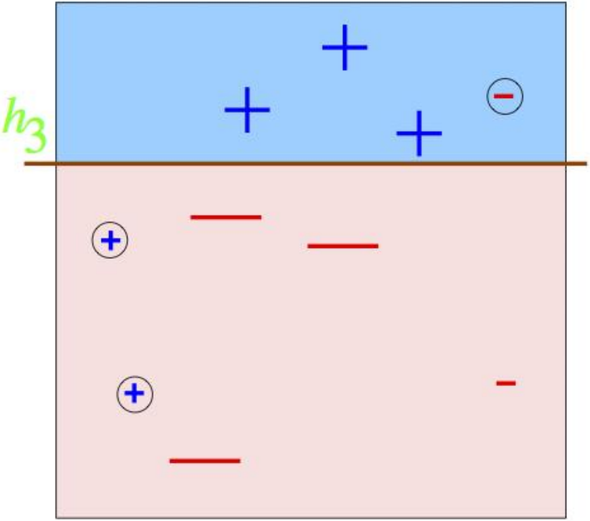
- Weak classifiers are horizontal and vertical lines
- Initial training data has equal weights
- First separator: vertical line
  - Increase weight of misclassified inputs
- Second separator: vertical line
  - Increase weight of misclassified inputs





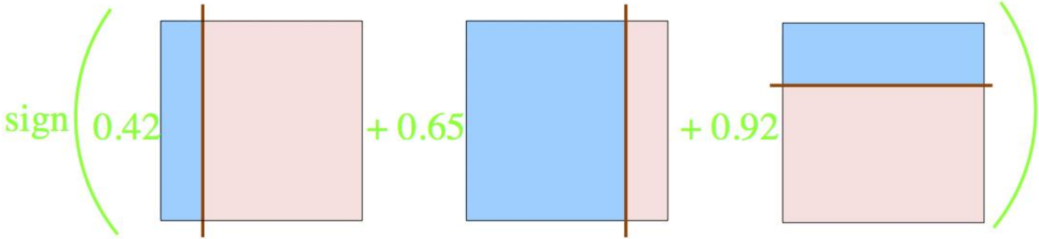
Boosting: An example

- Weak classifiers are horizontal and vertical lines
- Initial training data has equal weights
- First separator: vertical line
  - Increase weight of misclassified inputs
- Second separator: vertical line
  - Increase weight of misclassified inputs
- Third separator: horizontal line

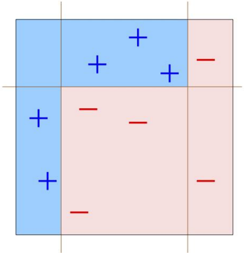


Boosting: An example

- Final classifier is weighted sum of three weak classifiers



- Pictorially



Gradient Boosting

- AdaBoost uses weights to build new weak learners that compensate for earlier errors
- Gradient boosting follows a different approach
  - Shortcomings of the current model are defined in terms of gradients
  - Gradient boosting = Gradient descent + boosting

Gradient Boosting for Regression

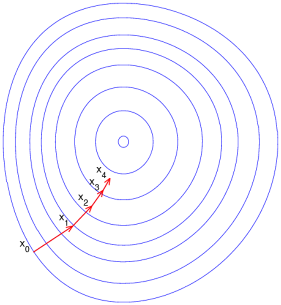
- Training data $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$
- Fit a model $F(x)$ to minimize square loss
- The model F we build is good, but not perfect
    - $y_1 = 0.9,\ F(x_1) = 0.8$
    - $y_2 = 1.3,\ F(x_2) = 1.4$
    - $\dots$
- Add an additional model h, so that new prediction is $F(x) + h(x)$
- What should h look like?
- For each x_i, want $F(x_i) + h(x_i) = y_i$
- $h(x_i) = y_i - F(x_i)$
- Fit a new model h (typically a regression tree) to the residuals $y_i - F(x_i)$
- If $F + h$ is not satisfactory, build another model h' to fit residuals $y_i - [F(x_i) + h(x_i)]$
- Why should this work?

Residuals and gradients

Gradient descent

- Move parameters against the gradient with respect to loss function

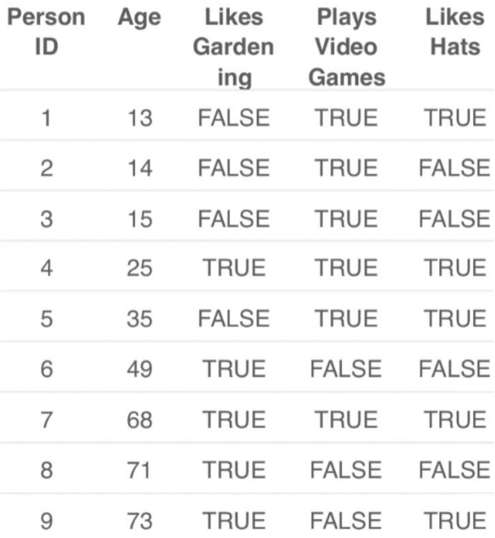
$$\theta_i \leftarrow \theta_i - \frac{\partial J}{\partial \theta_i}$$



- Individual loss:
  $L(y, F(x)) = (y - F(x))^2/2$
- Minimize overall loss:
  $J = \sum_i L(y_i, F(x_i))$
- $\dfrac{\partial J}{\partial F(x_i)} = F(x_i) - y$
- Residual $y_i - F(x_i)$ is negative gradient
- Fitting h to residual is same as fitting h to negative gradient
- Updating F using residual is same as updating F based on negative gradient

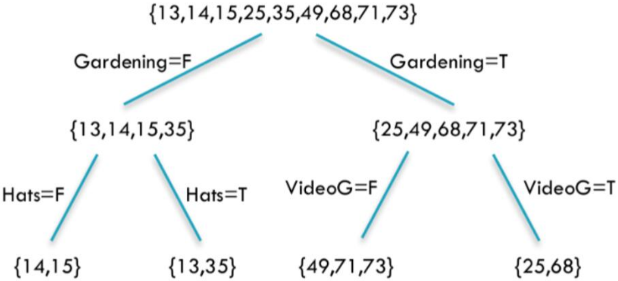
Regression Trees

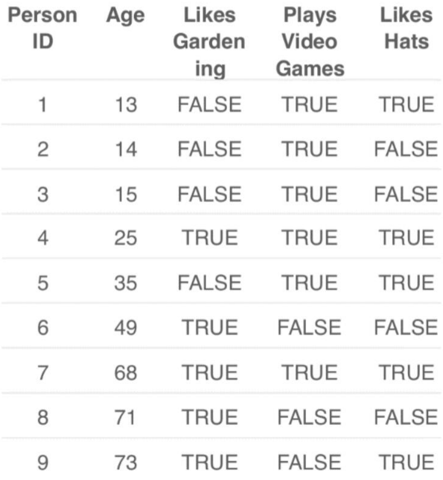
- Predict age based on given attributes
- Build a regression tree using CART algorithm



Person ID	Age	Likes Gardening	Plays Video Games	Likes Hats
1	13	FALSE	TRUE	TRUE
2	14	FALSE	TRUE	FALSE
3	15	FALSE	TRUE	FALSE
4	25	TRUE	TRUE	TRUE
5	35	FALSE	TRUE	TRUE
6	49	TRUE	FALSE	FALSE
7	68	TRUE	TRUE	TRUE
8	71	TRUE	FALSE	FALSE
9	73	TRUE	FALSE	TRUE

Regression Trees





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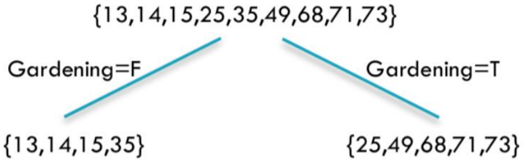
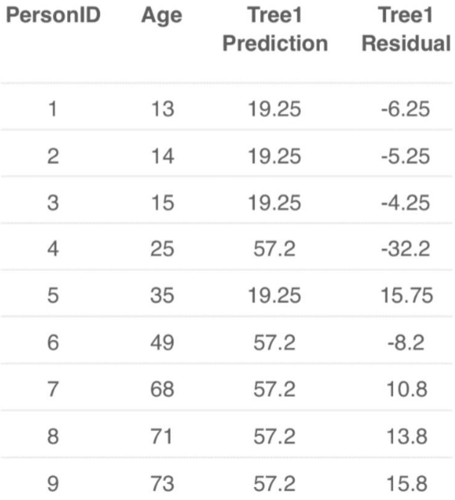
- **LikesHats** seems irrelevant, yet pops up
- Can we do better?

Residuals



Tree 1



PersonID	Age	Tree1 Prediction	Tree1 Residual
1	13	19.25	-6.25
2	14	19.25	-5.25
3	15	19.25	-4.25
4	25	57.2	-32.2
5	35	19.25	15.75
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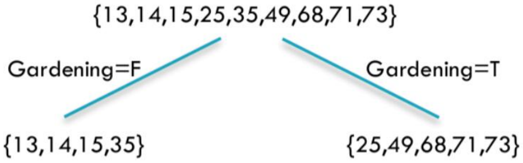

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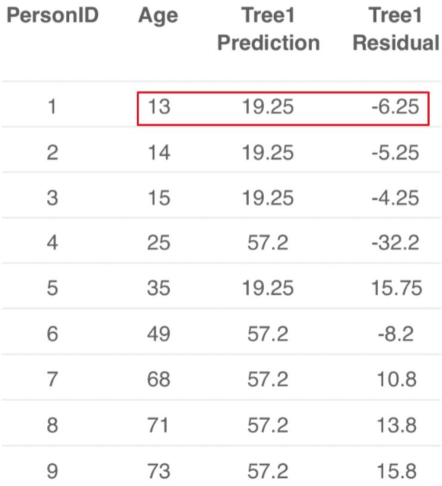

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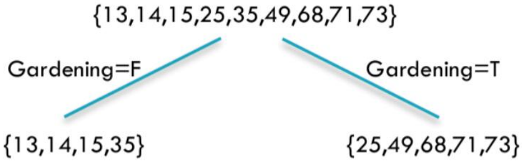

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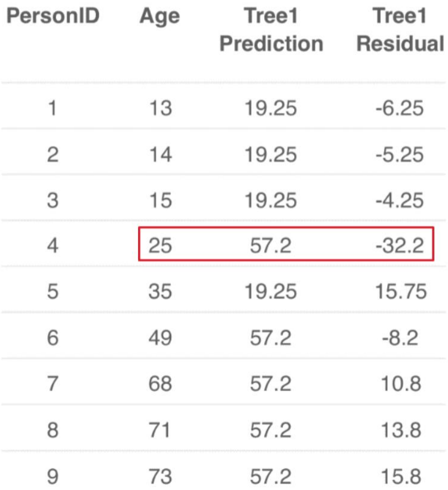

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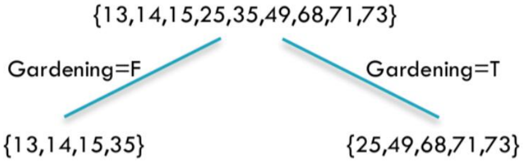
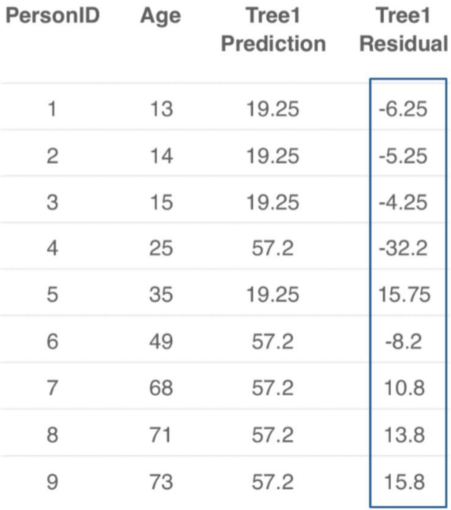


Tree 1



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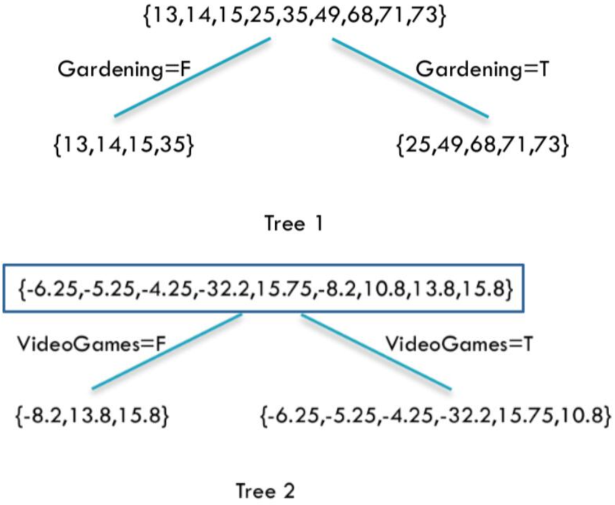


{13,14,15,25,35,49,68,71,73}

Gardening=F

Gardening=T

{13,14,15,35}

{25,49,68,71,73}

Tree 1

{-6.25,-5.25,-4.25,-32.2,15.75,-8.2,10.8,13.8,15.8}

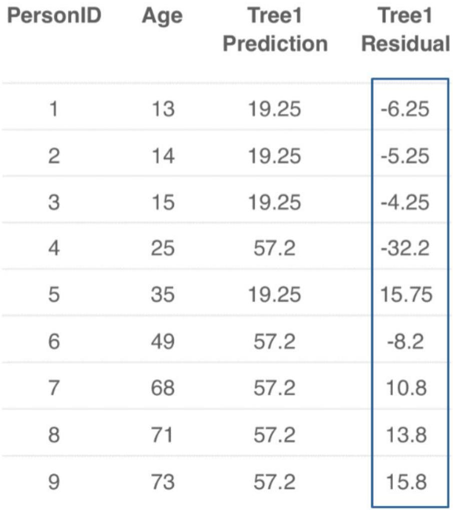
VideoGames=F

VideoGames=T

{-8.2,13.8,15.8}

{-6.25,-5.25,-4.25,-32.2,15.75,10.8}

Tree 2



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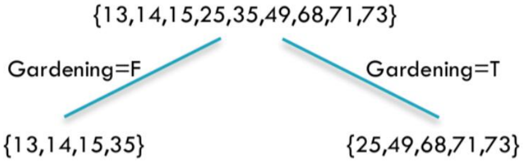

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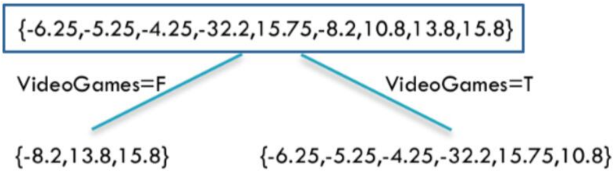
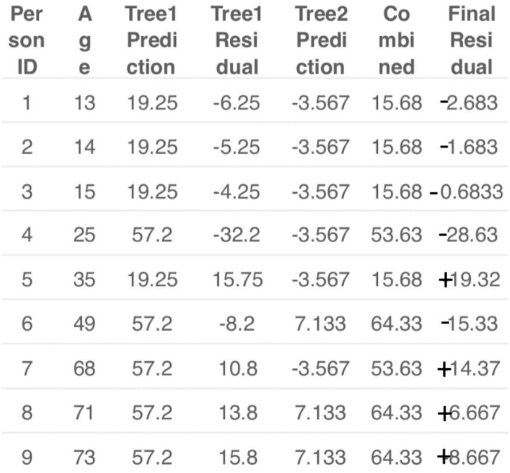
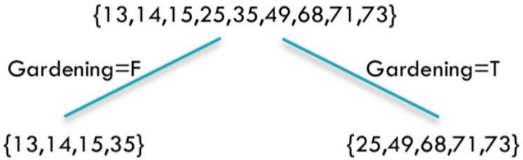


Tree 2



Person ID	Age	Tree1 Prediction	Tree1 Residual	Tree2 Prediction	Combined	Final Residual
1	13	19.25	-6.25	-3.567	15.68	-2.683
2	14	19.25	-5.25	-3.567	15.68	-1.683
3	15	19.25	-4.25	-3.567	15.68	-0.6833
4	25	57.2	-32.2	-3.567	53.63	-28.63
5	35	19.25	15.75	-3.567	15.68	+19.32
6	49	57.2	-8.2	7.133	64.33	-15.33
7	68	57.2	10.8	-3.567	53.63	+14.37
8	71	57.2	13.8	7.133	64.33	+6.667
9	73	57.2	15.8	7.133	64.33	+8.667

Residuals


{13,14,15,25,35,49,68,71,73}

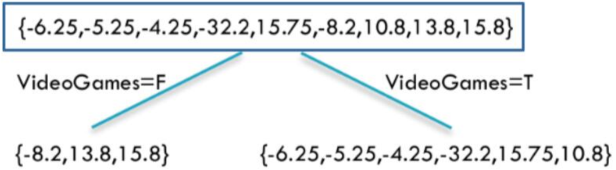
Gardening=F

Gardening=T

{13,14,15,35}

{25,49,68,71,73}

Tree 1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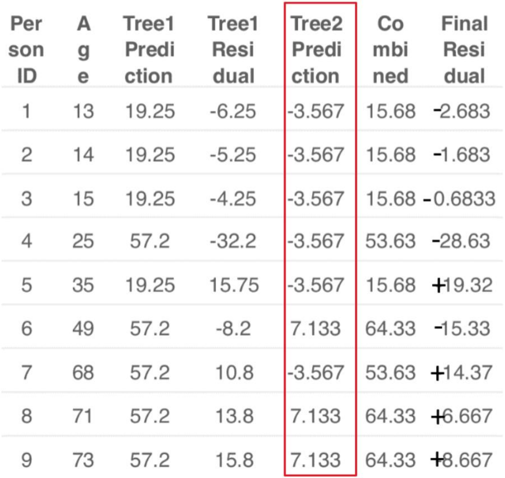
VideoGames=F

VideoGames=T

{-8.2,13.8,15.8}

{-6.25,-5.25,-4.25,-32.2,15.75,10.8}

Tree 2



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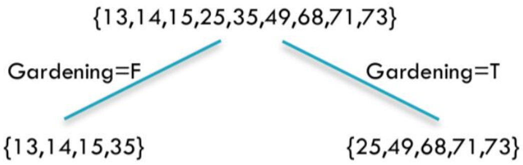
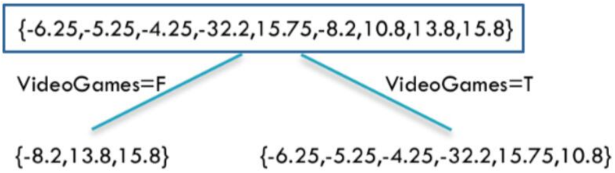
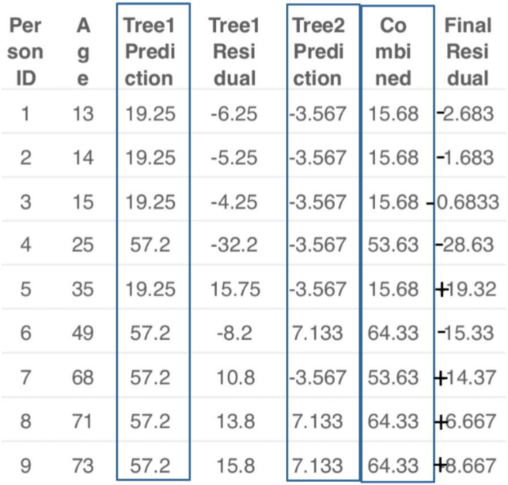
Residuals



Tree 1



Tree 2



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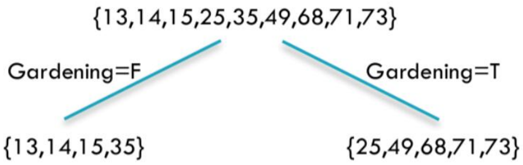
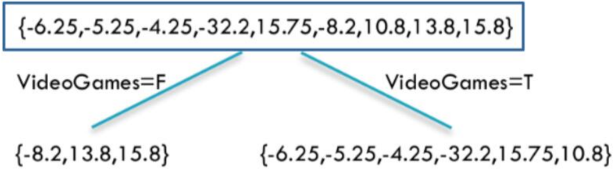
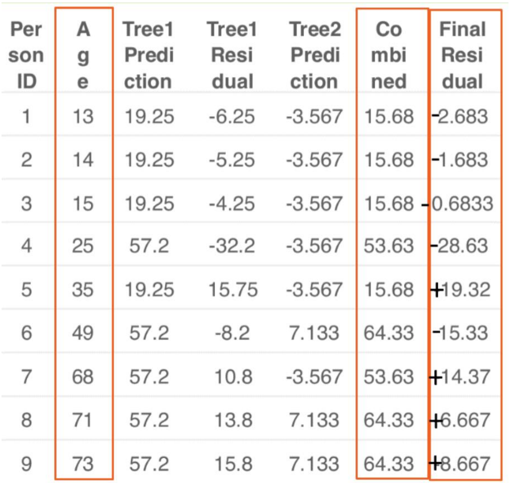
Residuals



Tree 1



Tree 2



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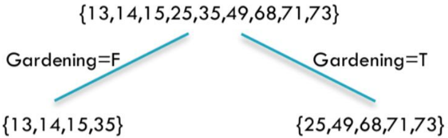
Gradient Boosting

General Strategy

- Build tree 1, F_1
- Fit a model to residuals, $h_1(x) = y - F_1(x)$
- Create a new model $F_2(x) = F_1(x) + h_1(x)$
- Fit a model to residuals, $h_2(x) = y - F_2(x)$
- Create a new model $F_3(x) = F_2(x) + h_2(x)$
- . . .



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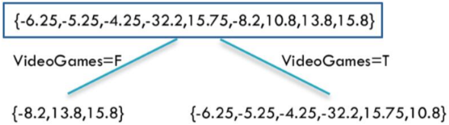
Gardening=F

Gardening=T

{13,14,15,35}

{25,49,68,71,73}

Tree 1



{-6.25,-5.25,-4.25,-32.2,15.75,-8.2,10.8,13.8,15.8}

VideoGames=F

VideoGames=T

{-8.2,13.8,15.8}

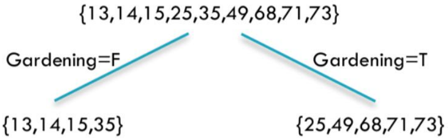
{-6.25,-5.25,-4.25,-32.2,15.75,10.8}

Tree 2

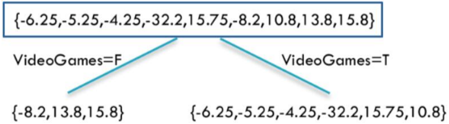
Hyper Parameters

Learning Rate

- h_j fits residuals of F_j
- $F_{j+1}(x) = F_J(x) + LR \cdot h_j(x)$
  - LR controls contribution of residual
  - $LR = 1$ in our previous example
- Ideally, choose LR separately for each residual to minimize loss function
  - Can apply different LR to different leaves



Tree 1



Tree 2

Residuals and gradients

- Residuals are a special case — gradients for square loss
- Can use other loss functions, and fit h to corresponding gradient
- Square loss gets skewed by outliers
- More robust loss functions with outliers
  - Absolute loss $|y - f(x)|$
  - Huber loss

$$L(y, F) = \begin{cases} \frac{1}{2}(y - F)^2, & |y - F| \leq \delta \\ \delta \cdot (|y - F| - \delta/2), & |y - F| > \delta \end{cases}$$

- More generally, boosting with respect to gradient rather than just residuals
- Given any differential loss function L,
  - Start with an initial model F
  - Calculate negative gradients

$$-g(x_i) = \frac{\partial L(y_i, F(x_i))}{\partial F(x_i)}$$

  - Fit a regression tree h to negative gradients $-g(x_i)$
  - Update F to $F + \rho h$
  - ρ is the learning rate

Gradient Boosting for Classification

- Assume binary classification
- Original training outputs are $y \in \{0,1\}$
- For each x, classifier produces scores $\langle s_0, s_1 \rangle$
- Use softmax to convert to probabilities:

  For $j \in \{0,1\}$, $p_j = \dfrac{e^{s_j}}{e^{s_0} + e^{s_1}}$
- Use cross entropy as the loss function

  $L(y, F) = y \log(p_1) + (1-y)\log(p_0)$
- Compute negative gradients
- Fit regression trees to negative gradients to minimize cross entropy