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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?

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

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

AdaBoost(D, Y, BaseLeaner, k)

Initialize $D_1(w_i) \leftarrow 1/n$ 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 $e_t > ½$ **then**

    $k \leftarrow k - 1$;

    exit-loop

  else

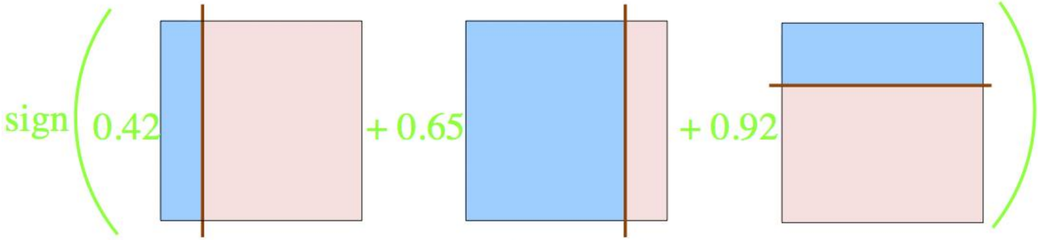
    $\beta_t \leftarrow e_t / (1 - e_t)$;

    $D_{t+1}(w_i) \leftarrow D_t(w_i) \times \begin{cases} \beta_t & \text{if } f_t(D_t(\mathbf{x}_i)) = y_i \\ 1 & \text{otherwise} \end{cases}$;

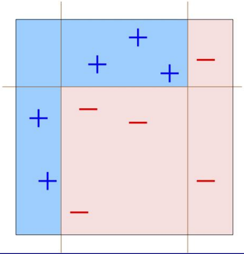
    $D_{t+1}(w_i) \leftarrow \dfrac{D_{t+1}(w_i)}{\sum_{i=1}^{n} D_{t+1}(w_i)}$

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

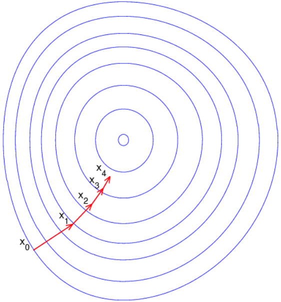
- Training data (x_1, y_1), (x_2, y_2), ..., (x_n, y_n)
- Fit a model $F(x)$ to minimize square loss
- The model F we build is good, but not perfect
  - $y_1 = 0.9$, $F(x_1) = 0.8$
  - $y_2 = 1.3$, $F(x_2) = 1.4$
  - ...
- Add an additional model h, so that new prediction is $F(x) + h(x)$
- What should 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

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

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

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

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

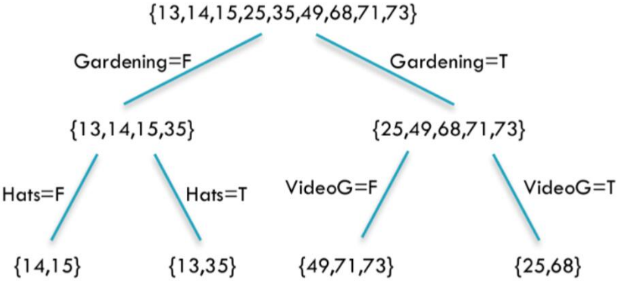
  - Fit a regression tree h to negative gradients $-g(x_i)$
  - Update F to $F + \rho h$
  - ρ is the learning rate

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

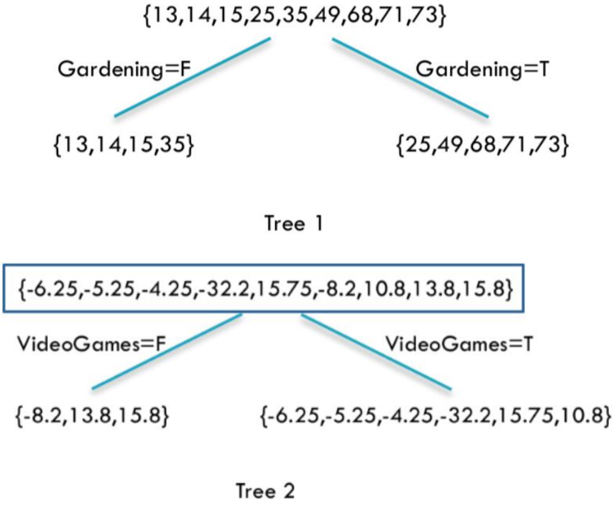
Regression Trees



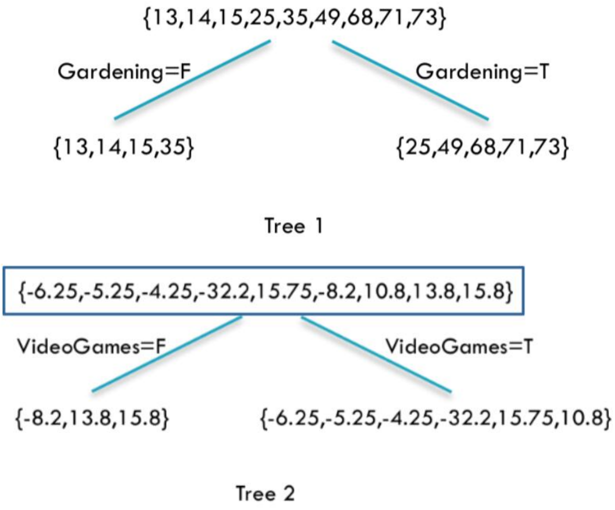
Person ID	Age	Likes Gardening	Plays Video Games	Likes Hats
1	13	FALSE	TRUE	TRUE
2	14	FALSE	TRUE	FALSE
3	15	FALSE	TRUE	FALSE
4	25	TRUE	TRUE	TRUE
5	35	FALSE	TRUE	TRUE
6	49	TRUE	FALSE	FALSE
7	68	TRUE	TRUE	TRUE
8	71	TRUE	FALSE	FALSE
9	73	TRUE	FALSE	TRUE

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

Residuals



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
6	49	57.2	-8.2
7	68	57.2	10.8
8	71	57.2	13.8
9	73	57.2	15.8

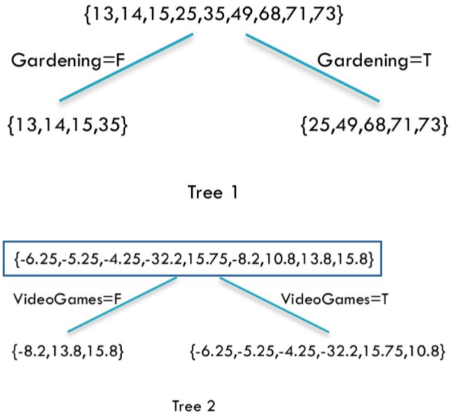


Person ID	Age	Tree1 Prediction	Tree1 Residual	Tree2 Prediction	Combined	Final Residual
1	13	19.25	-6.25	-3.567	15.68	-2.683
2	14	19.25	-5.25	-3.567	15.68	-1.683
3	15	19.25	-4.25	-3.567	15.68	-0.6833
4	25	57.2	-32.2	-3.567	53.63	-28.63
5	35	19.25	15.75	-3.567	15.68	+19.32
6	49	57.2	-8.2	7.133	64.33	-15.33
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

Gradient Boosting

General Strategy

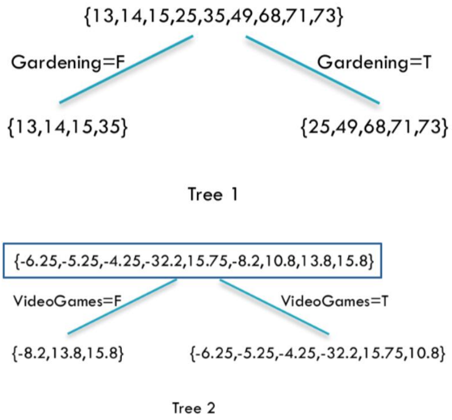
- Build tree 1, F_1
- Fit a model to residuals, $h_1(x) = y - F_1(x)$
- Create a new model $F_2(x) = F_1(x) + h_1(x)$
- Fit a model to residuals, $h_2(x) = y - F_2(x)$
- Create a new model $F_3(x) = F_2(x) + h_2(x)$
- ...



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



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