## Composite Models

Many methods can be see as:

E.g., neural networks, regression trees, random forest, ...

Some combinations don't help.

## Linear Models

Consider a generalized linear model

$$
\hat{Y}=f\left(w_{0}+w_{1} * F_{1} * \ldots w_{m} * F_{m}\right)
$$

## Linear Models

Consider a generalized linear model

$$
\hat{Y}=f\left(w_{0}+w_{1} * F_{1} * \ldots w_{m} * F_{m}\right)
$$

Where the the features $F_{i}$ come from?

## Linear Models

Consider a generalized linear model

$$
\hat{Y}=f\left(w_{0}+w_{1} * F_{1} * \ldots w_{m} * F_{m}\right)
$$

Where the the features $F_{i}$ come from?

- Input features.


## Linear Models

Consider a generalized linear model

$$
\hat{Y}=f\left(w_{0}+w_{1} * F_{1} * \ldots w_{m} * F_{m}\right)
$$

Where the the features $F_{i}$ come from?

- Input features.
- Boolean functions (e.g., using "and", "or", "equals", "greater than") of input features


## Linear Models

Consider a generalized linear model

$$
\hat{Y}=f\left(w_{0}+w_{1} * F_{1} * \ldots w_{m} * F_{m}\right)
$$

Where the the features $F_{i}$ come from?

- Input features.
- Boolean functions (e.g., using "and", "or", "equals", "greater than") of input features $\longrightarrow$ gradient boosted trees


## Linear Models

Consider a generalized linear model

$$
\hat{Y}=f\left(w_{0}+w_{1} * F_{1} * \ldots w_{m} * F_{m}\right)
$$

Where the the features $F_{i}$ come from?

- Input features.
- Boolean functions (e.g., using "and", "or", "equals", "greater than") of input features $\longrightarrow$ gradient boosted trees
- Piecewise linear functions of input features


## Linear Models

Consider a generalized linear model

$$
\hat{Y}=f\left(w_{0}+w_{1} * F_{1} * \ldots w_{m} * F_{m}\right)
$$

Where the the features $F_{i}$ come from?

- Input features.
- Boolean functions (e.g., using "and", "or", "equals", "greater than") of input features $\longrightarrow$ gradient boosted trees
- Piecewise linear functions of input features $\longrightarrow$ neural networks (with ReLU)


## Boosting

Boosting uses a sequence of learners where each one learns from the errors of the previous ones.

## Boosting

Boosting uses a sequence of learners where each one learns from the errors of the previous ones.
The features of a boosting algorithm are:

- There is a sequence of base learners e.g., small decision trees or (squashed) linear functions.


## Boosting

Boosting uses a sequence of learners where each one learns from the errors of the previous ones.
The features of a boosting algorithm are:

- There is a sequence of base learners e.g., small decision trees or (squashed) linear functions.
- Each learner is trained to fit the examples that the previous learners did not fit well.


## Boosting

Boosting uses a sequence of learners where each one learns from the errors of the previous ones.
The features of a boosting algorithm are:

- There is a sequence of base learners e.g., small decision trees or (squashed) linear functions.
- Each learner is trained to fit the examples that the previous learners did not fit well.
- The final prediction uses a mix (e.g., sum, weighted mean, or mode) of the predictions of each learner.


## Boosting

Boosting uses a sequence of learners where each one learns from the errors of the previous ones.
The features of a boosting algorithm are:

- There is a sequence of base learners e.g., small decision trees or (squashed) linear functions.
- Each learner is trained to fit the examples that the previous learners did not fit well.
- The final prediction uses a mix (e.g., sum, weighted mean, or mode) of the predictions of each learner.
The base learners can be weak learners.
They do not need to be very good; just better than random!


## Boosting

Boosting uses a sequence of learners where each one learns from the errors of the previous ones.
The features of a boosting algorithm are:

- There is a sequence of base learners e.g., small decision trees or (squashed) linear functions.
- Each learner is trained to fit the examples that the previous learners did not fit well.
- The final prediction uses a mix (e.g., sum, weighted mean, or mode) of the predictions of each learner.
The base learners can be weak learners.
They do not need to be very good; just better than random!
These weak learners are then boosted to be components in the ensemble that performs better than any of them.


## Functional Gradient Boosting for Regression

- Hyperparameter $K$ is the number of rounds of boosting.


## Functional Gradient Boosting for Regression

- Hyperparameter $K$ is the number of rounds of boosting.
- The final prediction is

$$
p_{0}+d_{1}(X)+\cdots+d_{K}(X)
$$

where $p_{0}$ is an initial prediction e.g., mean of training data.

## Functional Gradient Boosting for Regression

- Hyperparameter $K$ is the number of rounds of boosting.
- The final prediction is

$$
p_{0}+d_{1}(X)+\cdots+d_{K}(X)
$$

where $p_{0}$ is an initial prediction e.g., mean of training data.

- The ith prediction is

$$
p_{i}(X)=p_{0}+d_{1}(X)+\cdots+d_{i}(X)
$$

Then $p_{i}(X)=$

## Functional Gradient Boosting for Regression

- Hyperparameter $K$ is the number of rounds of boosting.
- The final prediction is

$$
p_{0}+d_{1}(X)+\cdots+d_{K}(X)
$$

where $p_{0}$ is an initial prediction e.g., mean of training data.

- The ith prediction is

$$
p_{i}(X)=p_{0}+d_{1}(X)+\cdots+d_{i}(X)
$$

Then $p_{i}(X)=p_{i-1}(X)+d_{i}(X)$.

## Functional Gradient Boosting for Regression (cont.)

- $p_{i}(X)=p_{i-1}(X)+d_{i}(X)$.


## Functional Gradient Boosting for Regression (cont.)

- $p_{i}(X)=p_{i-1}(X)+d_{i}(X)$.
- Each $d_{i}$ is constructed so that the error of $p_{i}$ is minimal, given that $p_{i-1}$ is fixed.


## Functional Gradient Boosting for Regression (cont.)

- $p_{i}(X)=p_{i-1}(X)+d_{i}(X)$.
- Each $d_{i}$ is constructed so that the error of $p_{i}$ is minimal, given that $p_{i-1}$ is fixed.
- At each stage, the base learner learns $\widehat{d}_{i}$ to minimize

$$
\sum_{e} \operatorname{loss}\left(p_{i-1}(e)+\widehat{d}_{i}(e), Y(e)\right)=\sum_{e} \operatorname{loss}\left(\widehat{d}_{i}(e), Y(e)-p_{i-1}(e)\right) .
$$

for any loss based on the difference between the actual and predicated value. (Which are these?)

## Functional Gradient Boosting for Regression (cont.)

- $p_{i}(X)=p_{i-1}(X)+d_{i}(X)$.
- Each $d_{i}$ is constructed so that the error of $p_{i}$ is minimal, given that $p_{i-1}$ is fixed.
- At each stage, the base learner learns $\widehat{d}_{i}$ to minimize

$$
\sum_{e} \operatorname{loss}\left(p_{i-1}(e)+\widehat{d}_{i}(e), Y(e)\right)=\sum_{e} \operatorname{loss}\left(\widehat{d}_{i}(e), Y(e)-p_{i-1}(e)\right) .
$$

for any loss based on the difference between the actual and predicated value. (Which are these?)

- The $i$ th learner learns $d_{i}(e)$ to fit $Y_{i}(e)-p_{i-1}(e)$.


## Functional Gradient Boosting for Regression (cont.)

- $p_{i}(X)=p_{i-1}(X)+d_{i}(X)$.
- Each $d_{i}$ is constructed so that the error of $p_{i}$ is minimal, given that $p_{i-1}$ is fixed.
- At each stage, the base learner learns $\widehat{d}_{i}$ to minimize

$$
\sum_{e} \operatorname{loss}\left(p_{i-1}(e)+\widehat{d}_{i}(e), Y(e)\right)=\sum_{e} \operatorname{loss}\left(\widehat{d}_{i}(e), Y(e)-p_{i-1}(e)\right)
$$

for any loss based on the difference between the actual and predicated value. (Which are these?)

- The $i$ th learner learns $d_{i}(e)$ to fit $Y_{i}(e)-p_{i-1}(e)$.

This is equivalent to learning from a modified dataset, where the previous prediction is subtracted from the actual value of the training set.

## Functional Gradient Boosting for Regression (cont.)

- $p_{i}(X)=p_{i-1}(X)+d_{i}(X)$.
- Each $d_{i}$ is constructed so that the error of $p_{i}$ is minimal, given that $p_{i-1}$ is fixed.
- At each stage, the base learner learns $\widehat{d}_{i}$ to minimize

$$
\sum_{e} \operatorname{loss}\left(p_{i-1}(e)+\widehat{d}_{i}(e), Y(e)\right)=\sum_{e} \operatorname{loss}\left(\widehat{d}_{i}(e), Y(e)-p_{i-1}(e)\right)
$$

for any loss based on the difference between the actual and predicated value. (Which are these?)

- The ith learner learns $d_{i}(e)$ to fit $Y_{i}(e)-p_{i-1}(e)$.

This is equivalent to learning from a modified dataset, where the previous prediction is subtracted from the actual value of the training set.

- Each learner is made to correct the errors of the previous prediction.


## Boosting_learner

1: procedure Boosting_learner $(X s, Y, E s, L, K)$
2: Inputs
$X s$ : set of input features; $Y$ : target feature; Es: training examples; $L$ : base learner; $K$ : number of components in the ensemble

## Output

function to make prediction on examples

## Boosting_learner

1: procedure Boosting_learner $(X s, Y, E s, L, K)$
2: Inputs
3: $\quad X s$ : set of input features; $Y$ : target feature; $E s$ : training examples; $L$ : base learner; $K$ : number of components in the ensemble

## Output

function to make prediction on examples
mean $:=\sum_{e \in E s} Y(e) /|E s|$
define $p_{0}(e)=$ mean

## Boosting_learner

1: procedure Boosting_learner $(X s, Y, E s, L, K)$
2: Inputs
3: $\quad X s$ : set of input features; $Y$ : target feature; $E s$ : training examples; $L$ : base learner; $K$ : number of components in the ensemble
4: Output
function to make prediction on examples
6: $\quad$ mean $:=\sum_{e \in E s} Y(e) /|E s|$
7: $\quad$ define $p_{0}(e)=$ mean
8: $\quad$ for each $i$ from 1 to $K$ do
9:

$$
\text { let } E_{i}=\left\{\left\langle X s(e), Y(e)-p_{i-1}(e)\right\rangle \text { for } e \in E s\right\}
$$

## Boosting_learner

1: procedure Boosting_learner $(X s, Y, E s, L, K)$
2: Inputs
3: $\quad X s$ : set of input features; $Y$ : target feature; $E s$ : training examples; $L$ : base learner; $K$ : number of components in the ensemble

## Output

function to make prediction on examples
mean $:=\sum_{e \in E_{s}} Y(e) /|E s|$
define $p_{0}(e)=$ mean
for each $i$ from 1 to $K$ do
let $E_{i}=\left\{\left\langle X s(e), Y(e)-p_{i-1}(e)\right\rangle\right.$ for $\left.e \in E s\right\}$
10: let $d_{i}=L\left(E_{i}\right) \quad \triangleright$ Learns function on examples given $\langle x, y\rangle$ pairs

## Boosting_learner

1: procedure Boosting_learner $(X s, Y, E s, L, K)$
2: Inputs
3: training examples; $L$ : base learner; $K$ : number of components in the ensemble

## Output

function to make prediction on examples
mean $:=\sum_{e \in E s} Y(e) /|E s|$
define $p_{0}(e)=$ mean
for each $i$ from 1 to $K$ do

$$
\text { let } E_{i}=\left\{\left\langle X s(e), Y(e)-p_{i-1}(e)\right\rangle \text { for } e \in E s\right\}
$$

10: $\quad$ let $d_{i}=L\left(E_{i}\right) \quad \triangleright$ Learns function on examples given $\langle x, y\rangle$ pairs
define $p_{i}(e)=p_{i-1}(e)+d_{i}(e)$

## Boosting_learner

1: procedure Boosting_learner $(X s, Y, E s, L, K)$
2: Inputs
3: training examples; $L$ : base learner; $K$ : number of components in the ensemble

## Output

function to make prediction on examples
mean $:=\sum_{e \in E_{s}} Y(e) /|E s|$
define $p_{0}(e)=$ mean
for each $i$ from 1 to $K$ do
let $E_{i}=\left\{\left\langle X s(e), Y(e)-p_{i-1}(e)\right\rangle\right.$ for $\left.e \in E s\right\}$
10: $\quad$ let $d_{i}=L\left(E_{i}\right) \quad \triangleright$ Learns function on examples given $\langle x, y\rangle$ pairs
define $p_{i}(e)=p_{i-1}(e)+d_{i}(e)$
return $p_{k}$

## Gradient-Boosted Trees

- Gradient-boosted trees are generalized linear models. The features are binary decision trees, learned using boosting.


## Gradient-Boosted Trees

- Gradient-boosted trees are generalized linear models. The features are binary decision trees, learned using boosting.
- For regression, the loss is regularized squared error:

$$
\left(\sum_{e}\left(\widehat{y_{e}}-y_{e}\right)^{2}\right)+\sum_{k=1}^{K} \Omega\left(f_{k}\right)
$$

The regularization is $\Omega(f)=\gamma *|w|+\frac{1}{2} \lambda * \sum_{j} w_{j}^{2}$, where $w$ is vector of weights. $\gamma$ and $\lambda$ are nonnegative numbers.

## Gradient-Boosted Trees

- Gradient-boosted trees are generalized linear models. The features are binary decision trees, learned using boosting.
- For regression, the loss is regularized squared error:

$$
\left(\sum_{e}\left(\widehat{y_{e}}-y_{e}\right)^{2}\right)+\sum_{k=1}^{K} \Omega\left(f_{k}\right)
$$

The regularization is $\Omega(f)=\gamma *|w|+\frac{1}{2} \lambda * \sum_{j} w_{j}^{2}$, where $w$ is vector of weights. $\gamma$ and $\lambda$ are nonnegative numbers.

- For Boolean classification, predict the sigmoid of sum of trees

$$
\widehat{y_{e}}=\operatorname{sigmoid}\left(\sum_{k=1}^{K} f_{k}\left(x_{e}\right)\right)
$$

## Gradient-Boosted Trees

- Gradient-boosted trees are generalized linear models. The features are binary decision trees, learned using boosting.
- For regression, the loss is regularized squared error:

$$
\left(\sum_{e}\left(\widehat{y_{e}}-y_{e}\right)^{2}\right)+\sum_{k=1}^{K} \Omega\left(f_{k}\right)
$$

The regularization is $\Omega(f)=\gamma *|w|+\frac{1}{2} \lambda * \sum_{j} w_{j}^{2}$, where $w$ is vector of weights. $\gamma$ and $\lambda$ are nonnegative numbers.

- For Boolean classification, predict the sigmoid of sum of trees

$$
\widehat{y_{e}}=\operatorname{sigmoid}\left(\sum_{k=1}^{K} f_{k}\left(x_{e}\right)\right)
$$

Optimize sum of log loss with the same regularization:

$$
\left(\sum_{e} \log \operatorname{loss}\left(\widehat{y_{e}}, y_{e}\right)\right)+\sum_{k=1}^{K} \Omega\left(f_{k}\right) .
$$

## Gradient-Boosted Trees

- Gradient-boosted trees, the tress are build sequentially: each tree is learned assuming the previous trees are fixed.


## Gradient-Boosted Trees

- Gradient-boosted trees, the tress are build sequentially: each tree is learned assuming the previous trees are fixed.
- Two issues:
- Selecting leaf values
- Selecting splits


## Gradient-Boosted Trees

- Gradient-boosted trees, the tress are build sequentially: each tree is learned assuming the previous trees are fixed.
- Two issues:
- Selecting leaf values
- Selecting splits
- For regression with squared error (or any loss based on the difference between the actual and predicated value), learn a tree for the difference between data and previous prediction.


## Selecting Leaf Values: Boolean Classification

- For the $t$ th tree, optimize log loss with $L 2$ regularization:

$$
\begin{aligned}
\widehat{y}_{e}^{(t)} & =\operatorname{sigmoid}\left(\sum_{k=1}^{t} f_{k}\left(x_{e}\right)\right) \\
\mathcal{L}^{(t)} & =\sum_{e} \log \operatorname{loss}\left(\widehat{y}_{e}^{(t)}, y_{e}\right)+\frac{1}{2} \lambda * \sum_{j} w_{j}^{2}+\text { constant }
\end{aligned}
$$

- Consider $j$ th leaf, where $I_{j}=\left\{e \mid q\left(x_{e}\right)=j\right\}$ is the set of training examples that map to it.
- Taking the derivative with respect to $w_{j}$ :

$$
\frac{\partial}{\partial w_{j}} \mathcal{L}^{(t)}=\lambda * w_{j}+\sum_{e \in I_{j}}\left(\widehat{y_{e}}-y_{e}\right)
$$

- A gradient descent step gives (Newton-Raphson method):

$$
w_{j}=\frac{\sum_{e \in I_{j}}\left(y_{e}-{\widehat{y_{e}}}^{(t-1)}\right)}{\sum_{e \in I_{j}}{\widehat{y_{e}}}^{(t-1)} *\left(1-\widehat{y e}^{(t-1)}\right)+\lambda}
$$

