Composite Models

Many methods can be see as:

$$\left.\begin{array}{r}\text{decision tree}\\ \text{logistic function}\\ \text{linear function}\\ \ldots\end{array}\right\} \text{ of } \left\{\begin{array}{l}\text{decision trees}\\ \text{logistic functions}\\ \text{linear functions}\\ \text{kernel functions}\\ \text{lower dimensional subspace}\\ \ldots\end{array}\right.$$

E.g., neural networks, regression trees, random forest, ...
Some combinations don't help.

Linear Models

Consider a generalized linear model

$$\hat{Y} = f(w_0 + w_1 * F_1 * \ldots w_m * F_m)$$

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.
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.
- 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.)

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

$$\sum_e loss(p_{i-1}(e)+\widehat{d}_i(e), Y(e)) = \sum_e loss(\widehat{d}_i(e), Y(e)-p_{i-1}(e)).$$

  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*(Xs, Y, Es, L, K)
2: **Inputs**
3: Xs: set of input features; Y: target feature; Es: training examples; L: base learner; K: number of components in the ensemble
4: **Output**
5: function to make prediction on examples
6: $mean := \sum_{e \in Es} Y(e)/|Es|$
7: define $p_0(e) = mean$
8: **for each** i from 1 to K **do**
9: let $E_i = \{\langle Xs(e), Y(e) - p_{i-1}(e)\rangle \text{ for } e \in Es\}$
10: let $d_i = L(E_i)$ ▷ Learns function on examples given $\langle x, y\rangle$ pairs
11: define $p_i(e) = p_{i-1}(e) + d_i(e)$
12: **return** p_k

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:

$$\left(\sum_e (\widehat{y_e} - y_e)^2\right) + \sum_{k=1}^{K} \Omega(f_k).$$

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

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

$$\widehat{y_e} = sigmoid(\sum_{k=1}^{K} f_k(x_e))$$

Optimize sum of log loss with the same regularization:

$$\left(\sum_e logloss(\widehat{y_e}, y_e)\right) + \sum_{k=1}^{K} \Omega(f_k).$$

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 tth tree, optimize log loss with $L2$ regularization:

$$\widehat{y_e}^{(t)} = sigmoid(\sum_{k=1}^{t} f_k(x_e))$$

$$\mathcal{L}^{(t)} = \sum_e logloss(\widehat{y_e}^{(t)}, y_e) + \frac{1}{2}\lambda * \sum_j w_j^2 + constant$$

- Consider jth leaf, where $I_j = \{e \mid q(x_e)=j\}$ is the set of training examples that map to it.
- Taking the derivative with respect to w_j:

$$\frac{\partial}{\partial w_j}\mathcal{L}^{(t)} = \lambda * w_j + \sum_{e \in I_j}(\widehat{y_e} - y_e)$$

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

$$w_j = \frac{\sum_{e \in I_j}(y_e - \widehat{y_e}^{(t-1)})}{\sum_{e \in I_j} \widehat{y_e}^{(t-1)} * (1 - \widehat{y_e}^{(t-1)}) + \lambda}$$