COMS30035, Machine learning: Combining Models 2, Ensembles

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Agenda

- Model Selection
- Model Averaging
- Ensembles: Bagging and Boosting
- Tree-based Models
- Conditional Mixture Models
- Ensembles of Humans

Ensemble Methods

- Ensemble: a combination of different models.
- The combination of models can often perform much better than the average individual, and sometimes better than the best individual.
- Different principle to BMA: the BMA weighted sum expresses uncertainty about which model is correct and tends to a single model as the dataset grows

Expected Error of an Ensemble

- Given a set of models, $1, ..., M$, take the mean of the individual predictions, $y_{COM} = \frac{1}{M}\sum_{m=1}^{M} y_m(\boldsymbol{x})$, where $y_m(\boldsymbol{x})$ is the prediction from model m.
- Let's compare the sum-of-squares error of y_{COM} with that of the individual models...
- Firstly, the expected error of our combination is:

$$E_{COM} = \mathbb{E}_{\boldsymbol{x}}[(y(\boldsymbol{x}) - y_{COM}(\boldsymbol{x}))^2] = \mathbb{E}_{\boldsymbol{x}}\left[\left(\frac{1}{M}\sum_{m=1}^{M} y(\boldsymbol{x}) - y_m(\boldsymbol{x})\right)^2\right]. \quad (1)$$

Expected Error of an Ensemble

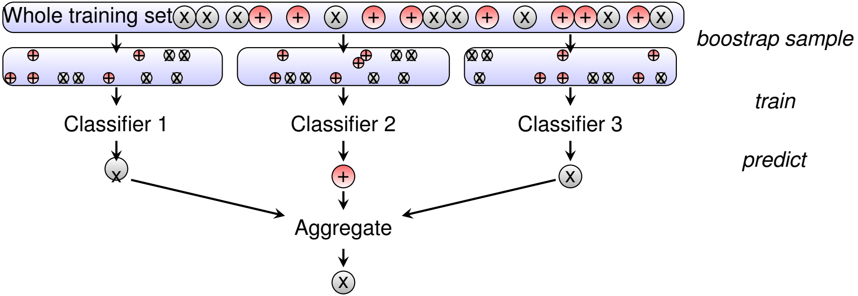
- $E_{COM} = \mathbb{E}_{\boldsymbol{x}}\left[\left(\frac{1}{M}\sum_{m=1}^{M} y(\boldsymbol{x}) - y_m(\boldsymbol{x})\right)^2\right]$.
- The average error of an individual model is: $E_{AV} = \frac{1}{M}\sum_{m=1}^{M} \mathbb{E}[(y(\boldsymbol{x}) - y_m(\boldsymbol{x}))^2]$.
- If we make two assumptions...
  1. The errors of each model have zero mean;
  2. The errors of different models are not correlated;
- ...then we arrive at $E_{COM} = \frac{1}{M}E_{AV}$!
- Intuition: if models make different, random errors, they will tend to cancel out.

Expected Error of an Ensemble

- $E_{COM} = \frac{1}{M} E_{AV}$ is pretty amazing, but is it realistic?
- No, because we have made extreme assumptions about the models' errors – in practice, they are usually highly correlated and biased.
- However, the combined error cannot be worse than the average error: $E_{COM} \leq E_{AV}$[1]
- The results tells us that the models should be *diverse* to avoid repeating the same errors.

[1] This bound is due to *Jensen's inequality*.

Bootstrap Aggregation (Bagging)



- Bagging is a simple ensemble method that induces diversity by training *M* models on different samples of the training set.
- For each model *m*, randomly sample *N* data points with replacement from a training set with *N* data points and train *m* on the subsample.
- In each bootstrap dataset, some data points will be repeated and others will be omitted.
- Combine predictions by taking the mean or majority vote.

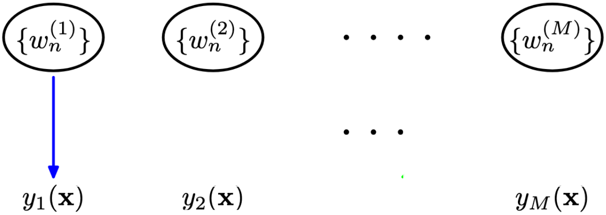
Boosting

- Can we do better than choosing training sets at random?
- We train the *base* models in sequence to ensure that each base model addresses the weaknesses of the ensemble.
- Instead of training a new base model on a random sample, weight the data points in the training set according to the performance of previous base models.
- *AdaBoost* is a popular boosting method for *binary classification*.

AdaBoost

Training sequence $\rightarrow$

train new classifier on weighted data that outputs class labels $+1$ or -1



$$Y_M(\mathbf{x}) = \text{sign}\left(\sum_m^M \alpha_m y_m(\mathbf{x}) \right)$$

AdaBoost

Training sequence $\rightarrow$

$\{w_n^{(1)}\}$ $\quad$ $\{w_n^{(2)}\}$ $\quad \cdot \cdot \cdot \cdot \quad$ $\{w_n^{(M)}\}$

$\cdot \cdot \cdot$

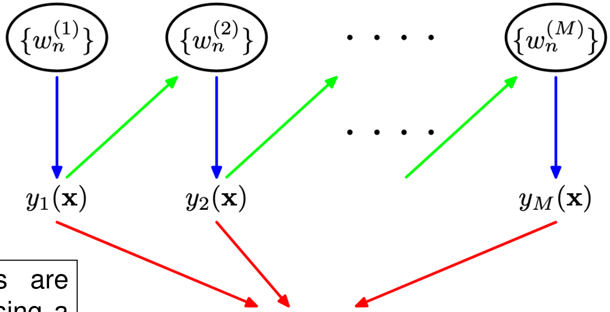
$y_1(\mathbf{x})$ $\quad$ $y_2(\mathbf{x})$ $\quad$ $y_M(\mathbf{x})$

compute weights from performance of previous classifier

$$Y_M(\mathbf{x}) = \text{sign}\left(\sum_m^M \alpha_m y_m(\mathbf{x})\right)$$

AdaBoost

Training sequence $\rightarrow$



after all classifiers are trained, combine using a weighted sum

$$Y_M(\mathbf{x}) = \text{sign}\left(\sum_m^M \alpha_m y_m(\mathbf{x})\right)$$

AdaBoost: Data Weights

1. Initialise to $1/N$;
2. Compute the weighted accuracy of model m:

$$\epsilon_m = \sum_{n=1}^{N} w_n^{(m)}[y_m(\boldsymbol{x}_n) \neq y(\boldsymbol{x}_n)] / \sum_{n=1}^{N} w_n^{(m)} \tag{2}$$

3. Update the weight for each data point n:

$$w_n^{(m+1)} = \begin{cases} w_n^{(m)} \left(\frac{1-\epsilon_m}{\epsilon_m}\right) & \text{if } y_m(\boldsymbol{x}_n) \neq y(\boldsymbol{x}_n) \\ w_n^{(m)} & \text{if } y_m(\boldsymbol{x}_n) = y(\boldsymbol{x}_n) \end{cases} \tag{3}$$

- The weight is increased when m makes an incorrect prediction.

AdaBoost: Final Classifier Weights

- AdaBoost chooses weight the α_m for m that minimises the exponential loss of base classifier m given previous classifiers:

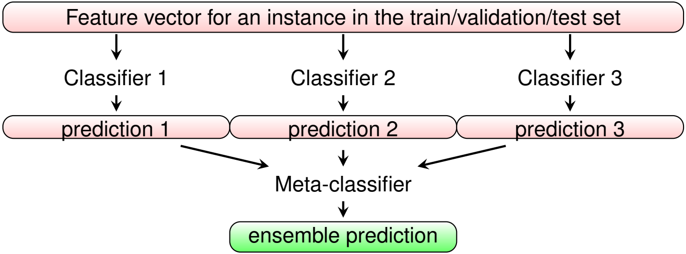
$$y_M(\boldsymbol{x}_n) = \sum_{m=1}^{M} \alpha_m y_m(\boldsymbol{x}_n), \tag{4}$$

$$\alpha_m = \ln\left\{\frac{1-\epsilon_m}{\epsilon_m}\right\} \tag{5}$$

- Weights are higher for classifiers with a lower error rate.
- Note that $alpha_m$ is a log-odds function: AdaBoost optimises the approximation to the log-odds ratio.
- Other loss functions can be used to derive similar boosting schemes for regression and multi-class classification.

Stacking

- Given a trained set of base classifiers, learn the combination function!
- For bagging, the combination function was just a majority vote which is an *unweighted* function;
- For Adaboost, we took a *weighted* sum of classifier outputs, where the weight of a base classifier is are determined from its individual error rate;
- Stacking uses another classifier to learn a combination of classifiers that minimises the error rate of the entire ensemble



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Now do the quiz!

Please do the quiz for this lecture on Blackboard.