COMS30035, Machine learning: Combining Models 2, Ensembles

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Agenda

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

Bayesian Model Averaging (BMA)

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- We can express uncertainty by assigning a probability to each model given the training data, $p(h|\boldsymbol{X})$.

Bayesian Model Averaging (BMA)

- Rather than choosing a single model, we can now take an expectation.
- Our predictions now come from a *weighted sum* over models, where $p(h|\boldsymbol{X})$ are weights :

$$p(\boldsymbol{z}|\boldsymbol{X}) = \sum_{h=1}^{H} p(\boldsymbol{z}|\boldsymbol{X}, h) p(h|\boldsymbol{X}) \quad (1)$$

Bayesian Model Averaging (BMA)

- Apply Bayes' rule to estimate the weights:

$$p(h|\boldsymbol{X}) = \frac{p(\boldsymbol{X}|h)p(h)}{\sum_{h'=1}^{H} p(\boldsymbol{X}|h')p(h')} \tag{2}$$

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- What happens as we increase the amount of data in $\boldsymbol{X}$?
- $p(h|\boldsymbol{X})$ becomes more focussed on one model.
- So BMA is soft model selection, it does not *combine* models to make a more powerful model.

Ensemble Methods

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- Model Averaging
- Ensembles: Bagging
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The combination was more effective than any one ‘model’.

Ensemble Methods

- Ensemble: a combination of different models.
- Often outperforms the average individual, and sometimes even the best individual.
- Different principle to BMA:
  - BMA weights try to identify a single, correct model
  - BMA weights do not provide the optimal combination

Expected Error of an Ensemble

- Given a set of models, $1, ..., M$,
- $y_m(\boldsymbol{x})$ is the prediction from model m.
- Simple ensemble: the mean of the individual predictions, $y_{COM} = \frac{1}{M} \sum_{m=1}^{M} y_m(\boldsymbol{x})$,

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- Simple ensemble: the mean of the individual predictions, $y_{COM} = \frac{1}{M}\sum_{m=1}^{M} y_m(\boldsymbol{x})$,
- Let's compare the sum-of-squares error of y_{COM} with that of the individual models...

Expected Error of an Ensemble

Firstly, the error of our combination for a particular input $\boldsymbol{x}$ is:

$$(y(\boldsymbol{x}) - y_{COM}(\boldsymbol{x}))^2 = \left(\frac{1}{M} \sum_{m=1}^{M} (y(\boldsymbol{x}) - y_m(\boldsymbol{x})) \right)^2 . \tag{3}$$

Expected Error of an Ensemble

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Expected Error of an Ensemble

- The expected error of an individual model m is: $E_m = \mathbb{E}_{\boldsymbol{x}}[(y(\boldsymbol{x}) - y_m(\boldsymbol{x}))^2]$.

Expected Error of an Ensemble

- The **average** expected error of an individual model is:
  $E_{AV} = \frac{1}{M} \sum_{m=1}^{M} \mathbb{E}_{\boldsymbol{x}} \left[(y(\boldsymbol{x}) - y_m(\boldsymbol{x}))^2 \right]$.

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  1. The errors of each model have zero mean;
  2. The errors of different models are not correlated;

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- This relies on two assumptions...
  1. The errors of each model have zero mean;
  2. The errors of different models are not correlated;
- Intuition: if models make different, random errors, they will tend to cancel out.

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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.

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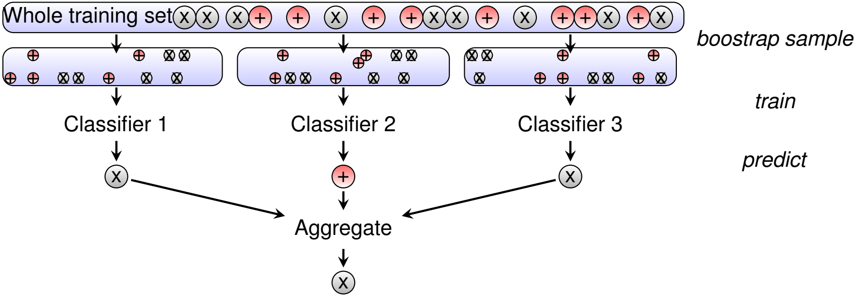
Bootstrap Aggregation (Bagging)



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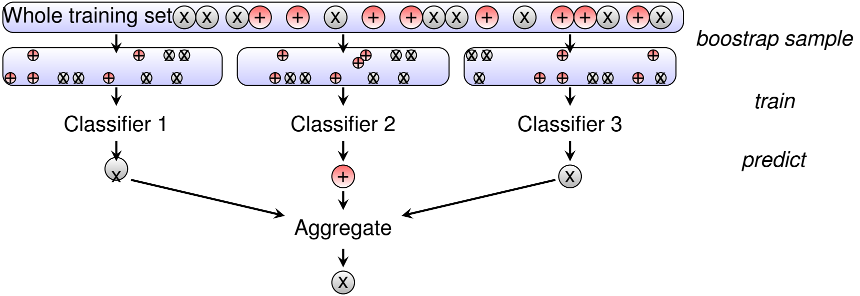

- Create diversity by training models on different samples of the training set.
- For each model *m*, randomly sample *N* data points with replacement from a training set with *N* data points and train *m* on the subsample.
- In each sample, some data points will be repeated and others will be omitted.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

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- Can we do better than choosing training sets at random?
- Train *base* models sequentially, ensuring that each base model addresses the weaknesses of the ensemble.
- Instead random sampling, weight the data points in the training set according to the performance of previous base models.
- *AdaBoost* is a popular boosting method originally designed for *binary classification*.

AdaBoost

Training sequence $\rightarrow$

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

$$\{w_n^{(1)}\}$$

$$\downarrow$$

$$y_1(\mathbf{x})$$

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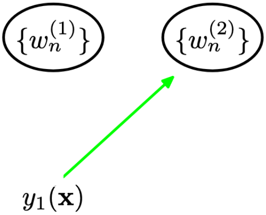
AdaBoost

Training sequence $\rightarrow$



compute weights from performance of previous classifier

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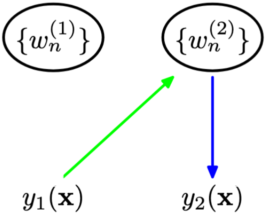

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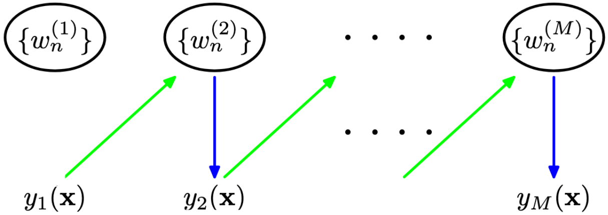

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$$\mathrm{n}\left(\sum_{m}^{M} \alpha_m y_m(\mathbf{x})\right)$$

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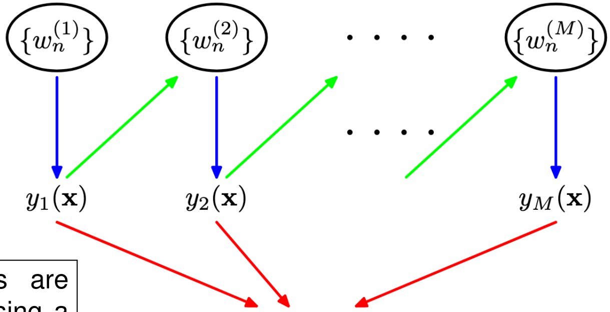

after all classifiers are trained, combine using a weighted sum

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

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3. Update the weight for each data point n:

$$w_n^{(m+1)} = \begin{cases} w_n^{(m)} \left(\frac{1-\epsilon_m}{\epsilon_m}\right) & \text{if } y_m(\boldsymbol{x}_n) \neq y(\boldsymbol{x}_n) \\ w_n^{(m)} & \text{if } y_m(\boldsymbol{x}_n) = y(\boldsymbol{x}_n) \end{cases} \tag{6}$$

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

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- Note that α_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 set of trained base classifiers, what's the best way to combine them?

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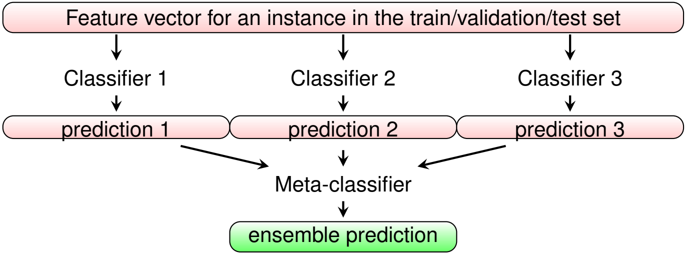

Now do the quiz!

Please do the quiz for this lecture on Blackboard.