COMS30035, Machine learning: Combining Models 1, Selecting and Combining

Edwin Simpson
edwin.simpson@bristol.ac.uk

Department of Computer Science, SCEEM
University of Bristol

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Agenda

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

Textbook

We will follow Chapter 14 of the Bishop book: Bishop, C. M., Pattern recognition and machine learning (2006). Available for free here.

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  - Parameters of the learning algorithm, like learning rate for stochastic gradient descent (SGD);
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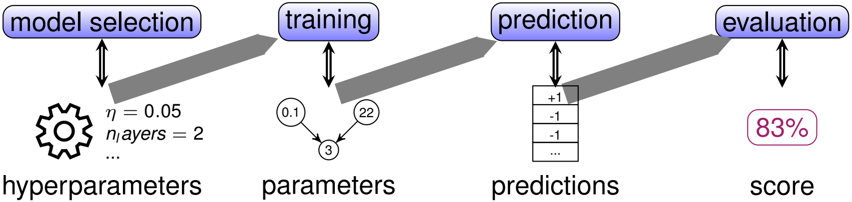
  - The examples in the dataset the model is trained on;
  - Random initialisation of parameters for EM or SGD

Hyperparameters



- It's useful to characterise all of these modelling decisions as *hyperparameters*
- Hyperparameters = all modelling choices that are fixed before training

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- Weakness: if the validation set is small, we might choose the wrong model!

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- How do we come up with *H*?
- Random search: test random combinations of hyperparameters
- Grid search: For each hyperparameter, define a set of values to test
  - Use your knowledge of the problem to test only reasonable values
  - For numerical hyperparameters, e.g., learning rate, choose a set of evenly-spaced values within a sensible range
  - *H* contains all combinations of the chosen hyperparameter values

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  - H contains all combinations of the chosen hyperparameter values
- Reduce the number of tests needed to find a good combination using a more intelligent strategy such as Bayesian Optimisation

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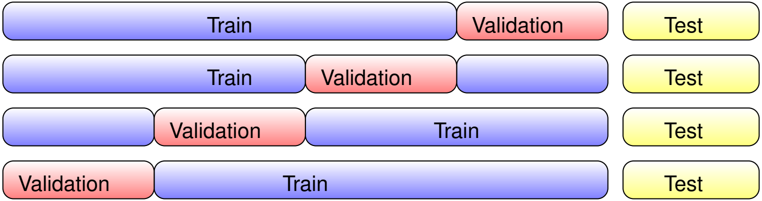
Cross-validation



- Split the training data into k random, equally-sized subsets;
- For each of the k folds: leave out the kth subset from training, train on the rest and test on the kth subset;
- Compute the average performance across all k folds;
- Avoids overfitting by tuning on training set performance...
- And avoids tuning on a single small validation set.

A Probabilistic View of Model Selection

- Suppose we have the following machine learning task:
  - Latent variables to predict (e.g., class labels in the test set): $\boldsymbol{z}$;
  - Observed data: $\boldsymbol{X}$;
  - Model: h.
- We obtain the prediction of $\boldsymbol{z}$ from a chosen model h as follows:

$$p(\boldsymbol{z}|\boldsymbol{X}) \approx p(\boldsymbol{z}|\boldsymbol{X}, h) \tag{1}$$

Bayesian Model Selection

- How can we choose h in $p(\boldsymbol{z}|\boldsymbol{X}, h)$?
- Choose $h = h^*$ to *maximise* the marginal likelihood of the data:

$$h^* = \underset{h}{\operatorname{argmax}} p(\boldsymbol{X}|h) = \underset{h}{\operatorname{argmax}} \int p(\boldsymbol{X}|\boldsymbol{\theta}, h) p(\boldsymbol{\theta}|h) d\boldsymbol{\theta} \tag{2}$$

- Similar to maximum likelihood estimation, which we used before to optimise parameters $\boldsymbol{\theta}$.
  - Here, we use a Bayesian approach and integrate out (marginalise) $\boldsymbol{\theta}$.
  - Relies on finding a single, good model given our training set.

Bayesian Model Averaging (BMA)

- Even after computing marginal likelihood, we may be uncertain about which model h is correct
- We can express this 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 :

$$p(\boldsymbol{z}|\boldsymbol{X}) = \sum_{h=1}^{H} p(\boldsymbol{z}|\boldsymbol{X}, h)p(h|\boldsymbol{X}) \tag{3}$$

Bayesian Model Averaging (BMA)

- Apply Bayes' rule to estimate the weights:

$$p(h|\boldsymbol{X}) = \frac{p(\boldsymbol{X}|h)p(h)}{\sum_{h'=1}^{H} p(\boldsymbol{X}|h)p(h')} \quad (4)$$

- 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

Wisdom of the crowd

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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:

$$(y(\boldsymbol{x}) - y_{COM}(\boldsymbol{x}))^2 = \left(\frac{1}{M} \sum_{m=1}^{M} y(\boldsymbol{x}) - y_m(\boldsymbol{x}) \right)^2 . \tag{5}$$

Expected Error of an Ensemble

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$$E_{COM} = \mathbb{E}_{\boldsymbol{x}}[(y(\boldsymbol{x}) - y_{COM}(\boldsymbol{x}))^2] = \mathbb{E}_{\boldsymbol{x}}\left[\left(\frac{1}{M}\sum_{m=1}^{M}(y(\boldsymbol{x}) - y_m(\boldsymbol{x}))\right)^2\right]. \quad (6)$$

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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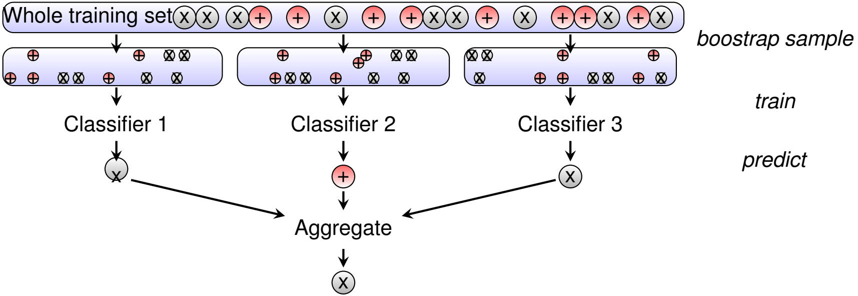
- ...so we have $E_{COM} = \frac{1}{M}E_{AV}$, since for E_{COM}, the $\frac{1}{M}$ is squared
- Intuition: if models make different, random errors, they will tend to cancel out.

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)



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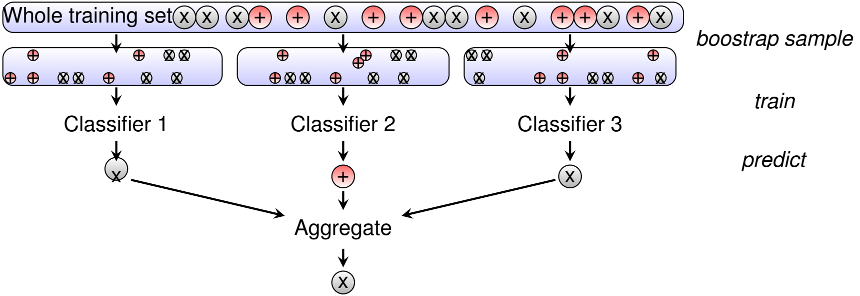

- Create diversity by training models on different samples of the training set.
- For each model *m*, randomly sample *N* data points with replacement from a training set with *N* data points and train *m* on the subsample.
- In each sample, some data points will be repeated and others will be omitted.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

Now do the quiz!

Please do the quiz for this lecture on Blackboard.