Ensemble Methods

The rationale

- Groups of individuals can make better decisions than individuals (if they don't all think the same)
- Combining multiple ML models can produce better predictions than those of any single model
- Training ensembles can (often) be parallelized, with substantial computational savings

Note
Models should be diverse enough for the ensemble to work

How to guarantee diversity?

Ensembling strategies

bagging diversify the training sets

stacking diversify the models being trained

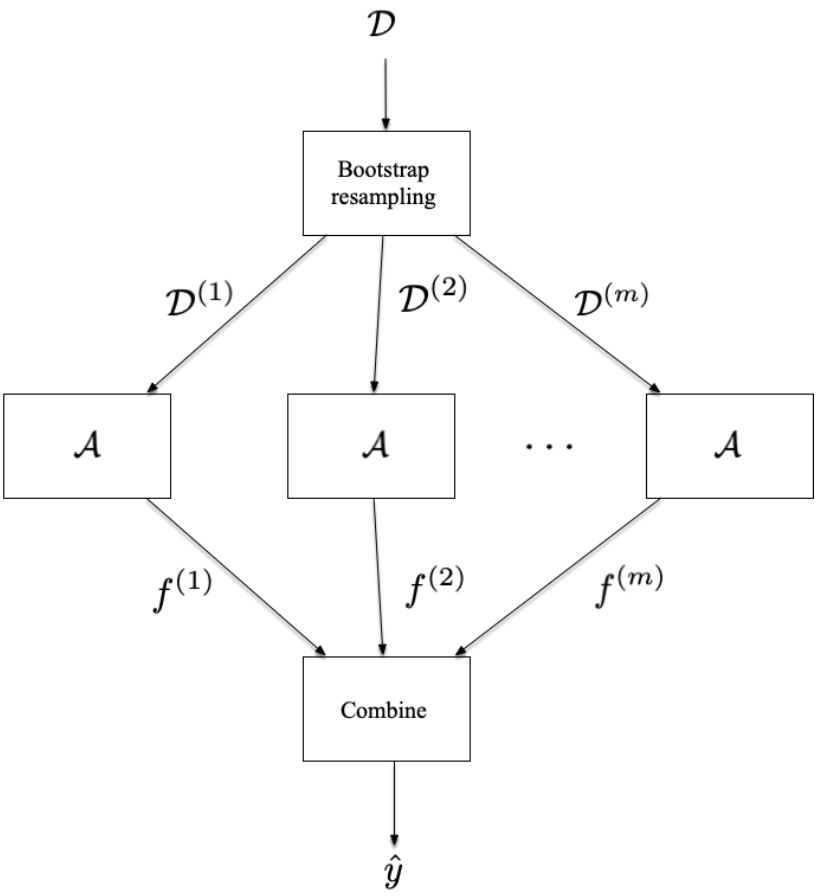
boosting (progressively) diversify the importance of examples

Bagging: Bootstrap aggregation

In a nutshell

- Take a learning algorithm $\mathcal{A}$ (e.g. decision tree learning)
- Extract m different datasets $\mathcal{D}^{(i)}$ from the original training set $\mathcal{D}$
- Train one base model per dataset
$$f^{(i)} = \mathcal{A}(\mathcal{D}^{(i)})$$
- Combine predictions of different base models
$$\hat{y} = \textsc{Combine}(f^{(1)}(x), \ldots, f^{(m)}(x))$$

Bagging: Bootstrap aggregation



Bagging: Bootstrap aggregation

Extracting datasets: boostrap resampling

- Simply partitioning $\mathcal{D}$ into m subsets produces very small training sets
- *Bootstrap resampling* extracts $N = |\mathcal{D}|$ samples from $\mathcal{D}$ *with replacement* (i.e., same example can be selected multiple times)
- Repeating the procedure m times to get diverse datasets of the same size as $\mathcal{D}$

Bagging: Bootstrap aggregation

Diversity of Datasets

- Each example has probability $(1 - 1/N)$ of not being selected at each draw
- Each example has probability $(1 - 1/N)^N$ of not being selected after N draws
- For large enough N, this is 37%, i.e., 37% of the dataset are not part of a given training set (*out-of-bag instances*, oob)
- oob instances can be used to estimate test performance of the base model

Bagging: Bootstrap aggregation

Combination strategies

Majority voting predict the class with most votes (classification)

$$\hat{y} = argmax_y \sum_{i=1}^{m} \delta(y, \hat{y}^{(i)})$$

Soft voting predict the class with largest sum of predicted probability (classification). Assumes base classifier outputs a confidence/probability

$$\hat{y} = argmax_y \sum_{i=1}^{m} f_y^{(i)}(x)$$

Mean predict the mean (or median) of the base model outputs (regression)

$$\hat{y} = \sum_{i=1}^{m} f^{(i)}(x)$$

Bagging example: Random forests

Bagging + model decorrelation

- Use decision trees as the base models
- Even if $\mathcal{D}^{(i)} \neq \mathcal{D}^{(j)}$, the learned DTs can be too much correlated
- Introduce additional stochasticity in the DT training process
- At each node, choose the best feature to split from a random selection of the set of features (instead of using them all)

Stacking: stacked generalization

In a nutshell

- Train m base models $f^{(i)}$ on $\mathcal{D}$ with m *different* learning algorithms $\mathcal{A}^{(i)}$

$$f^{(i)} = \mathcal{A}^{(i)}(\mathcal{D})$$

- Use a *meta-learner* to learn to combine base models (e.g., linear combination)

$$g = \mathcal{A}_{META}([f^{(1)}, \ldots, f^{(m)}], \mathcal{D}')$$

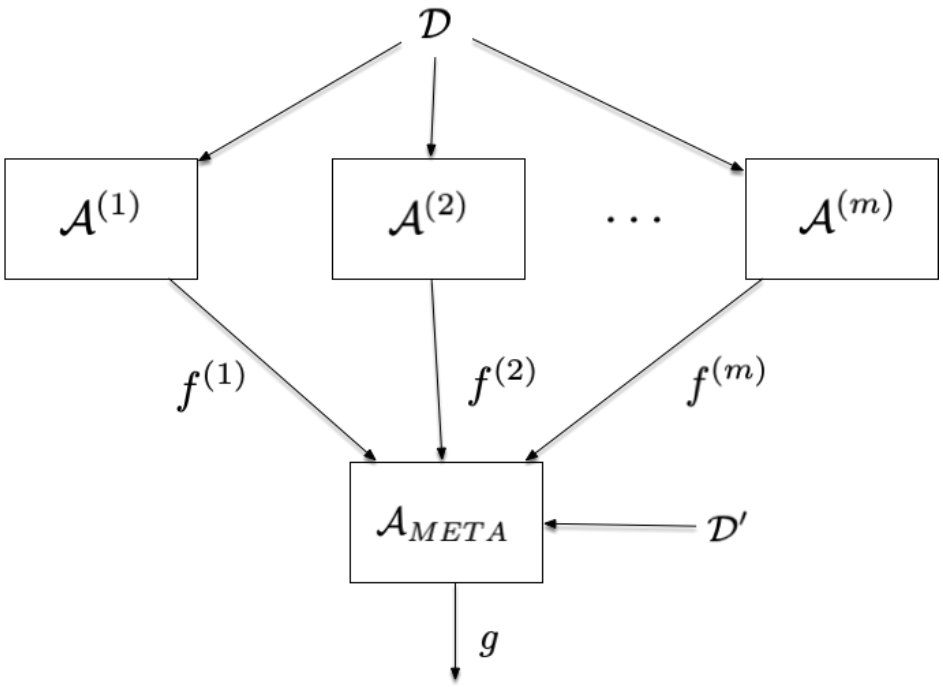
- Use the meta-model to output ensemble predictions

$$\hat{y} = g\left([f^{(1)}(x), \ldots, f^{(m)}(x)]\right)$$

Note

The meta-model should be trained on a dataset $\mathcal{D}' \neq \mathcal{D}$, or it will learn to focus on the best performing model on $\mathcal{D}$.

Stacking: stacked generalization



Boosting

In a nutshell

- Take a learner $\mathcal{A}$ and train it on $\mathcal{D}$
- Reweight examples in $\mathcal{D}$ based on their accuracy according to the trained model (harder examples get larger weights)
- Train $\mathcal{A}$ again on the reweighted dataset
- Repeat the procedure m times
- Combine the learned models into the final model

Boosting weak learners

From weak learners to strong learners

- A *weak learner* learns models with accuracy slightly better than random.
- A weak learner is easy to implement and train.
- Applying boosting with weak learners as the base learning algorithm allows to turn them into *strong learners*
- This can be easier than designing a strong learner directly.

Boosting example: AdaBoost

procedure ADABOOST
  $\mathbf{d}^{(0)} \leftarrow \langle \frac{1}{N}, \ldots, \frac{1}{N} \rangle$ ▷ initialize importance weights uniformly
  for $i = 1, \ldots, m$ **do**
    $f^{(i)} \leftarrow \mathcal{A}(\mathcal{D}, \mathbf{d}^{(i-1)})$ ▷ train i^{th} model on weighted data
    $\hat{y}_n \leftarrow f^{(i)}(x_n), \forall n$ ▷ collect model predictions
    $\hat{\epsilon}^{(i)} \leftarrow \sum_n d_n^{(i-1)} \mathbb{1}[y_n \neq \hat{y}_n]$ ▷ compute weighted training error
    $\alpha^{(i)} \leftarrow \frac{1}{2} \log\left(\frac{1-\hat{\epsilon}^{(i)}}{\hat{\epsilon}^{(i)}}\right)$ ▷ compute adaptive parameter
    $d_n^{(i)} \leftarrow \frac{1}{Z} d_n^{(i-1)} \exp(-\alpha^{(i)} y_n \hat{y}_n), \forall n$ ▷ re-weight examples
  end for
  return $f(\mathbf{x}) = \text{sgn}(\sum_i \alpha^{(i)} f^{(i)}(\mathbf{x}))$ ▷ return ensemble model
end procedure

AdaBoost

$$d_n^{(i)} \leftarrow \frac{1}{Z} d_n^{(i-1)} \exp(-\alpha^{(i)} y_n \hat{y}_n)$$

Example re-weighting

- correctly classified examples $y_n \hat{y}_n = +1$ are multiplicatively downweighted
- incorrectly classified examples $y_n \hat{y}_n = -1$ are multiplicatively upweighted
- Z is a normalization constant making weights sum to one (importance as probability distribution over examples)

AdaBoost

Role of adaptive parameter (1)

- Let $\mathcal{D}$ have 80 positive and 20 negative examples
- Assume the first classifier $f^{(1)}$ simply returns the majority class (i.e., $f^{(1)}(\mathbf{x}_n) = +1$ for all n)
- It's weighted error rate is 0.2 (all negative examples are incorrectly predicted)
- The adaptive parameter is
$$\alpha^{(1)} = \frac{1}{2} \log\left(\frac{1-\hat{\epsilon}^{(i)}}{\hat{\epsilon}^{(i)}}\right) = 1/2 \log(4)$$
- The multiplicative weight for positive (correct) examples is $\exp(-\alpha^{(i)} y_n \hat{y}_n) = \exp(-1/2 \log(4)) = 1/2$.
- The multiplicative weight for negative (incorrect) examples is $\exp(-\alpha^{(i)} y_n \hat{y}_n) = \exp(1/2 \log(4)) = 2$.

AdaBoost

Role of adaptive parameter (2)

- The normalization Z (ignoring $d_n^{(i-1)}$ for simplicity) is $80 * 1/2 + 20 * 2 = 80$
- the normalized weights for positive and negative examples are $1/2 * 1/80 = 1/160$ and $2 * 1/80 = 1/40$
- The overall weight of positive and negative examples is now $1/160 * 80 = 1/2$ and $1/40 * 20 = 1/2$
- The reweighted dataset is thus fully balanced, and a majority class predictor is not a weak learner any more (accuracy exactly 50%).

References

- H. Daume. *A Course in Machine Learning*, http://ciml.info/
- K. Murphy, Probabilistic Machine Learning: An Introduction, The MIT Press, 2021 (online version at https://probml.github.io/pml-book/book1.html)