Classification

Ensemble

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Outline

1 Intro

2 Bagging

3 Boosting

4 Random Forests

Ensemble Methods

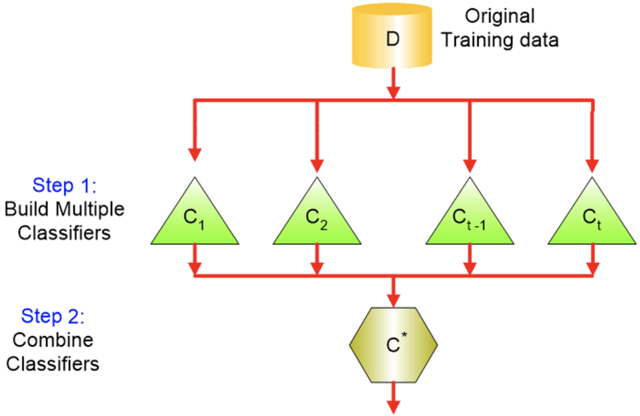
- Construct a **set of classifiers** from the training data
- Predict class label of test records by **combining the predictions made by multiple classifiers**

Why Ensemble Methods work?

- Suppose there are 25 base classifiers
  - Each classifier has error rate $\epsilon = 0.35$
  - Assume errors made by classifiers are uncorrelated
  - Probability that the ensemble classifier makes a wrong prediction:

$$P(X \geq 13) = \sum_{i=13}^{25} \binom{25}{i} \epsilon^i (1-\epsilon)^{25-i} = 0.06$$

General Approach



Types of Ensemble Methods

- Manipulate data distribution
  - Example: bagging, boosting
- Manipulate input features
  - Example: random forests

Bagging

- Bootstrap aggregating (Bagging)
- Sampling with replacement

Original data	1	2	3	4	5	6	7	8	9	10
Bagging (round 1)	7	8	10	8	2	5	10	10	5	9
Bagging (round 2)	1	4	9	1	2	3	2	7	3	2
Bagging (round 3)	1	8	5	10	5	5	9	6	3	7

- Build classifier on **each bootstrap sample**
- Each sample has probability $1-(1-\frac{1}{n})^n$ of being selected. If n is sufficiently large, this probability converges to $1-\frac{1}{e} \approx 0.632$
  Proof: `https://juanitorduz.github.io/bootstrap/`

Bagging Algorithm

Algorithm 4.5 Bagging algorithm.

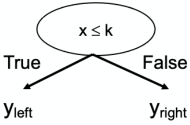
1: Let k be the number of bootstrap samples.
2: **for** $i = 1$ to k **do**
3: Create a bootstrap sample of size N, D_i.
4: Train a base classifier C_i on the bootstrap sample D_i.
5: **end for**
6: $C^*(x) = \underset{y}{\operatorname{argmax}} \sum_i \delta\big(C_i(x) = y\big)$.
$\{\delta(\cdot) = 1$ if its argument is true and 0 otherwise.$\}$

Bagging Example

- Consider 1-dimensional data set:

x	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
y	1	1	1	-1	-1	-1	-1	1	1	1

- Classifier is a decision stump (one-level binary decision tree)
  - Decision rule: $x \leq k$ versus $x > k$
  - Split point k is chosen based on entropy



Bagging Example (cont.)

Bagging Round 1:

x	0.1	0.2	0.2	0.3	0.4	0.4	0.5	0.6	0.9	0.9
y	1	1	1	1	-1	-1	-1	-1	1	1

x <= 0.35 → y = 1
x > 0.35 → y = -1

Bagging Example (cont.)

Bagging Round 1:

x	0.1	0.2	0.2	0.3	0.4	0.4	0.5	0.6	0.9	0.9
y	1	1	1	1	-1	-1	-1	-1	1	1

x <= 0.35 → y = 1
x > 0.35 → y = -1

Bagging Round 2:

x	0.1	0.2	0.3	0.4	0.5	0.5	0.9	1	1	1
y	1	1	1	-1	-1	-1	1	1	1	1

x <= 0.7 → y = 1
x > 0.7 → y = 1

Bagging Round 3:

x	0.1	0.2	0.3	0.4	0.4	0.5	0.7	0.7	0.8	0.9
y	1	1	1	-1	-1	-1	-1	-1	1	1

x <= 0.35 → y = 1
x > 0.35 → y = -1

Bagging Round 4:

x	0.1	0.1	0.2	0.4	0.4	0.5	0.5	0.7	0.8	0.9
y	1	1	1	-1	-1	-1	-1	-1	1	1

x <= 0.3 → y = 1
x > 0.3 → y = -1

Bagging Round 5:

x	0.1	0.1	0.2	0.5	0.6	0.6	0.6	1	1	1
y	1	1	1	-1	-1	-1	-1	1	1	1

x <= 0.35 → y = 1
x > 0.35 → y = -1

Bagging Example (cont.)

Bagging Round 6:

x	0.2	0.4	0.5	0.6	0.7	0.7	0.7	0.8	0.9	1
y	1	-1	-1	-1	-1	-1	-1	1	1	1

x <= 0.75 → y = -1
x > 0.75 → y = 1

Bagging Round 7:

x	0.1	0.4	0.4	0.6	0.7	0.8	0.9	0.9	0.9	1
y	1	-1	-1	-1	-1	1	1	1	1	1

x <= 0.75 → y = -1
x > 0.75 → y = 1

Bagging Round 8:

x	0.1	0.2	0.5	0.5	0.5	0.7	0.7	0.8	0.9	1
y	1	1	-1	-1	-1	-1	-1	1	1	1

x <= 0.75 → y = -1
x > 0.75 → y = 1

Bagging Round 9:

x	0.1	0.3	0.4	0.4	0.6	0.7	0.7	0.8	1	1
y	1	1	-1	-1	-1	-1	-1	1	1	1

x <= 0.75 → y = -1
x > 0.75 → y = 1

Bagging Round 10:

x	0.1	0.1	0.1	0.1	0.3	0.3	0.8	0.8	0.9	0.9
y	1	1	1	1	1	1	1	1	1	1

x <= 0.05 → y = 1
x > 0.05 → y = 1

Bagging Example (cont.)

- Summary of Training sets

Round	Split Point	Left Class	Right Class
1	0.35	1	-1
2	0.7	1	1
3	0.35	1	-1
4	0.3	1	-1
5	0.35	1	-1
6	0.75	-1	1
7	0.75	-1	1
8	0.75	-1	1
9	0.75	-1	1
10	0.05	1	1

Bagging Example (cont.)

- Assume test set is the same as the original data
- Use majority vote to determine class of ensemble classifier

Round	x=0.1	x=0.2	x=0.3	x=0.4	x=0.5	x=0.6	x=0.7	x=0.8	x=0.9	x=1.0
1	1	1	1	-1	-1	-1	-1	-1	-1	-1
2	1	1	1	1	1	1	1	1	1	1
3	1	1	1	-1	-1	-1	-1	-1	-1	-1
4	1	1	1	-1	-1	-1	-1	-1	-1	-1
5	1	1	1	-1	-1	-1	-1	-1	-1	-1
6	-1	-1	-1	-1	-1	-1	-1	1	1	1
7	-1	-1	-1	-1	-1	-1	-1	1	1	1
8	-1	-1	-1	-1	-1	-1	-1	1	1	1
9	-1	-1	-1	-1	-1	-1	-1	1	1	1
10	1	1	1	1	1	1	1	1	1	1
Sum	2	2	2	-6	-6	-6	-6	2	2	2
Sign	1	1	1	-1	-1	-1	-1	1	1	1

Predicted Class

Boosting

- An iterative procedure to adaptively change distribution of training data by focusing more on **previously misclassified records**
  - Initially, all N records are assigned equal weights
  - Unlike bagging, weights may change at the end of each boosting round

Boosting

- Records that are wrongly classified will have their weights increased
- Reords that are classified correctly will have their weights decreased

Original Data	1	2	3	4	5	6	7	8	9	10
Boosting (Round 1)	7	3	2	8	7	9	4	10	6	3
Boosting (Round 2)	5	4	9	4	2	5	1	7	4	2
Boosting (Round 3)	4	4	8	10	4	5	4	6	3	4

  - Suppose example 4 is hard to classify
  - Its weight is increased, therefore it is more likely to be chosen again in subsequent rounds

AdaBoost

- Adaptive Boosting (AdaBoost) is a common implementation of the boosting method.
- Base classifiers: $C_1, C_2, \cdots, C_T$

Error rate = (# of instances that are wrongly classied)/N
= \sum (\delta)/N

- Error rate of class C_i

$$\epsilon_i = \frac{1}{N}\sum_{j=1}^{N} w_j \delta(C_i(\mathbf{x}_j) \neq y_j)$$

Text

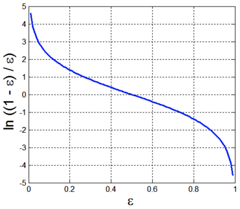
Here, $\delta(p) = 1$ if the predicate p is true, and 0 otherwise.

- Importance of a classifier C_i

$\alpha_i = \frac{1}{2} ln \left(\frac{1-\epsilon_i}{\epsilon_i}\right)$,

- α_i has a large positive value if ϵ_i is close to 0

- α_i has a large negative value if ϵ_i is close to 1, as shown in the right figure.



AdaBoost Algorithm

- Weight update (Eq. 4.103)

$$w_i^{(j+1)} = \frac{w_i^{(j)}}{Z_j} \cdot \begin{cases} exp^{-\alpha_j} & \text{if } C_j(\mathbf{x}_i) = y_i \\ exp^{\alpha_j} & \text{if } C_j(\mathbf{x}_i) \neq y_i \end{cases}$$

where $Z_j = \sum_{i=1}^{N} w_i^{(j)}$ is the normalization factor.

- If any intermediate rounds produce error rate higher than 50%, the weights are reverted back to $\frac{1}{n}$ and the resampling procedure is repeated
- Classification:

$$C^*(\mathbf{x}) = argmax_y \sum_{j=1}^{T} \alpha_j \delta(C_j(\mathbf{x}) = y)$$

AdaBoost Algorithm (cont.)

Algorithm 4.6 AdaBoost algorithm.

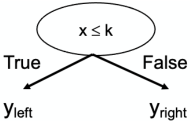
1: $\mathbf{w} = \{w_j = 1/N \mid j = 1, 2, \ldots, N\}$. {Initialize the weights for all N examples.}
2: Let k be the number of boosting rounds.
3: **for** $i = 1$ to k **do**
4: Create training set D_i by sampling (with replacement) from D according to $\mathbf{w}$.
5: Train a base classifier C_i on D_i.
6: Apply C_i to all examples in the original training set, D.
7: $\epsilon_i = \frac{1}{N}\left[\sum_j w_j \, \delta\big(C_i(x_j) \neq y_j\big)\right]$ {Calculate the weighted error.}
8: **if** $\epsilon_i > 0.5$ **then**
9: $\mathbf{w} = \{w_j = 1/N \mid j = 1, 2, \ldots, N\}$. {Reset the weights for all N examples.}
10: Go back to Step 4.
11: **end if**
12: $\alpha_i = \frac{1}{2} \ln \frac{1-\epsilon_i}{\epsilon_i}$.
13: Update the weight of each example according to Equation 4.103.
14: **end for**
15: $C^*(\mathbf{x}) = \underset{y}{\operatorname{argmax}} \sum_{j=1}^{T} \alpha_j \delta\big(C_j(\mathbf{x}) = y\big)$.

AdaBoost Example

- Consider 1-dimensional data set:

x	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
y	1	1	1	-1	-1	-1	-1	1	1	1

- Classifier is a decision stump (one-level binary decision tree)
  - Decision rule: $x \leq k$ versus $x > k$
  - Split point k is chosen based on entropy



AdaBoost Example (cont.)

- Training sets for the first 3 boosting rounds:

Boosting Round 1:

x	0.1	0.4	0.5	0.6	0.6	0.7	0.7	0.7	0.8	1
y	1	-1	-1	-1	-1	-1	-1	-1	1	1

Boosting Round 2:

x	0.1	0.1	0.2	0.2	0.2	0.2	0.3	0.3	0.3	0.3
y	1	1	1	1	1	1	1	1	1	1

Boosting Round 3:

x	0.2	0.2	0.4	0.4	0.4	0.4	0.5	0.6	0.6	0.7
y	1	1	-1	-1	-1	-1	-1	-1	-1	-1

- Summary

Round	Split Point	Left Class	Right Class	alpha
1	0.75	-1	1	1.738
2	0.05	1	1	2.7784
3	0.3	1	-1	4.1195

AdaBoost Example (cont.)

- Weights

Round	x=0.1	x=0.2	x=0.3	x=0.4	x=0.5	x=0.6	x=0.7	x=0.8	x=0.9	x=1.0
1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
2	0.311	0.311	0.311	0.01	0.01	0.01	0.01	0.01	0.01	0.01
3	0.029	0.029	0.029	0.228	0.228	0.228	0.228	0.009	0.009	0.009

- Classification

0

Round	x=0.1	x=0.2	x=0.3	x=0.4	x=0.5	x=0.6	x=0.7	x=0.8	x=0.9	x=1.0
1	-1	-1	-1	-1	-1	-1	-1	1	1	1
2	1	1	1	1	1	1	1	1	1	1
3	1	1	1	-1	-1	-1	-1	-1	-1	-1
Sum	5.16	5.16	5.16	-3.08	-3.08	-3.08	-3.08	0.397	0.397	0.397
Sign	1	1	1	-1	-1	-1	-1	1	1	1

Predicted Class

Random Forests

- Build on the idea of bagging to use a different bootstrap sample of the training data for learning decision trees.

- Key difference: the best splitting criterion is chosen from **a small set of randomly selected attributes**.

Training a random forest classifier

- Construct a **bootstrap sample** D_i of the training set by randomly **sampling** n **instances** (with replacement) from D.
- Use D_i to learn a decision tree T_i as follows: At every internal node of T_i, randomly sample **a set of** p **attributes** and choose an attribute from this subset for splitting.
- The final prediction of the random forest is based on **majority voting**.

Empirical Comparison among Ensemble Methods

Data Set	Number of (Attributes, Classes, Records)	Decision Tree (%)	Bagging (%)	Boosting (%)	RF (%)
Anneal	(39, 6, 898)	92.09	94.43	95.43	95.43
Australia	(15, 2, 690)	85.51	87.10	85.22	85.80
Auto	(26, 7, 205)	81.95	85.37	85.37	84.39
Breast	(11, 2, 699)	95.14	96.42	97.28	96.14
Cleve	(14, 2, 303)	76.24	81.52	82.18	82.18
Credit	(16, 2, 690)	85.8	86.23	86.09	85.8
Diabetes	(9, 2, 768)	72.40	76.30	73.18	75.13
German	(21, 2, 1000)	70.90	73.40	73.00	74.5
Glass	(10, 7, 214)	67.29	76.17	77.57	78.04
Heart	(14, 2, 270)	80.00	81.48	80.74	83.33
Hepatitis	(20, 2, 155)	81.94	81.29	83.87	83.23
Horse	(23, 2, 368)	85.33	85.87	81.25	85.33
Ionosphere	(35, 2, 351)	89.17	92.02	93.73	93.45
Iris	(5, 3, 150)	94.67	94.67	94.00	93.33
Labor	(17, 2, 57)	78.95	84.21	89.47	84.21
Led7	(8, 10, 3200)	73.34	73.66	73.34	73.06
Lymphography	(19, 4, 148)	77.03	79.05	85.14	82.43
Pima	(9, 2, 768)	74.35	76.69	73.44	77.60
Sonar	(61, 2, 208)	78.85	78.85	84.62	85.58
Tic-tac-toe	(10, 2, 958)	83.72	93.84	98.54	95.82
Vehicle	(19, 4, 846)	71.04	74.11	78.25	74.94
Waveform	(22, 3, 5000)	76.44	83.30	83.90	84.04
Wine	(14, 3, 178)	94.38	96.07	97.75	97.75
Zoo	(17, 7, 101)	93.07	93.07	95.05	97.03

References

- Chapter 4: Introduction to Data Mining (2nd Edition) by Pang-Ning Tan, Michael Steinbach, Anuj Karpatne, and Vipin Kumar
- Python Scikit-learn Bagging Classifier `https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.BaggingClassifier.html`
- Python Scikit-learn AdaBoost Classifier `https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.AdaBoostClassifier.html`
- Python Scikit-learn Random Forests `https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.RandomForestClassifier.html`