10701
Machine Learning

Ensemble methods and Boosting
Fighting the bias-variance tradeoff

• **Simple (a.k.a. weak) learners are good**
  – e.g., naïve Bayes, logistic regression, decision stumps (or shallow decision trees)
  – Low variance, don’t usually overfit

• **Simple (a.k.a. weak) learners are bad**
  – High bias, can’t solve hard learning problems

• Can we make all weak learners always good???
  – No!!
  – But often yes...
Simplest approach: A “bucket of models”

• Input:
  – your top $T$ favorite learners (or tunings)
    • $L_1, \ldots, L_T$
  – A dataset $D$

• Learning algorithm:
  – Use 10-CV to estimate the error of $L_1, \ldots, L_T$
  – Pick the best (lowest 10-CV error) learner $L^*$
  – Train $L^*$ on $D$ and return its hypothesis $h^*$
Pros and cons of a “bucket of models”

• Pros:
  – Simple
  – Will give results not much worse than the best of the “base learners”

• Cons:
  – What if there’s not a single best learner?

• Other approaches:
  – Vote the hypotheses (how would you weight them?)
  – Combine them some other way?
  – How about learning to combine the hypotheses?
Stacked learners: first attempt

• Input:
  – your top $T$ favorite learners (or tunings)
    • $L_1, \ldots, L_T$
  – A dataset $D$ containing $(x,y)$, ....

• Learning algorithm:
  – Train $L_1, \ldots, L_T$ on $D$ to get $h_1, \ldots, h_T$
  – Create a new dataset $D'$ containing $(x',y')$, ....
    • $x'$ is a vector of the $T$ predictions $h_1(x), \ldots, h_T(x)$
    • $y$ is the label $y$ for $x$
  – Train new classifier on $D'$ to get $h'$ --- which combines the predictions!

• To predict on a new $x$:
  – Construct $x'$ as before and predict $h'$ ($x'$)
Pros and cons of stacking

• Pros:
  – Fairly simple
  – Slow, but easy to parallelize

• Cons:
  – What if there’s not a single best combination scheme?
  – E.g.: for movie recommendation sometimes L1 is best for users with many ratings and L2 is best for users with few ratings.
Voting (Ensemble Methods)

• Instead of learning a single (weak) classifier, learn many weak classifiers that are good at different parts of the input space

• Output class: (Weighted) vote of each classifier
  – Classifiers that are most “sure” will vote with more conviction
  – Classifiers will be most “sure” about a particular part of the space
  – On average, do better than single classifier!

• But how do you ???
  – force classifiers to learn about different parts of the input space?
  – weigh the votes of different classifiers?
Comments

• Ensembles based on blending/stacking were key approaches used in successful applications (for example, the Netflix competition)
  – Winning entries blended many types of classifiers

• Ensembles based on stacking are the main architecture used in Watson
  – Not all of the base classifiers/rankers are learned, however; some are hand-programmed.
Boosting [Schapire, 1989]

- Idea: given a weak learner, run it multiple times on (rewighted) training data, then let the learned classifiers vote

- On each iteration $t$:
  - weight each training example by how incorrectly it was classified
  - Learn a hypothesis $- h_t$
  - A strength for this hypothesis $- \alpha_t$

- Final classifier:
  - A linear combination of the votes of the different classifiers weighted by their strength

- Practically useful
- Theoretically interesting
Learning from weighted data

• Sometimes not all data points are equal
  – Some data points are more equal than others
• Consider a weighted dataset
  – \( D(i) \) – weight of \( i \) th training example \((x^i, y^i)\)
  – Interpretations:
    • \( i \) th training example counts as \( D(i) \) examples
    • If I were to “resample” data, I would get more samples of “heavier” data points

• Now, in all calculations, whenever used, \( i \) th training example counts as \( D(i) \) “examples”
  – e.g., MLE for Naïve Bayes, redefine \( \text{Count}(Y=y) \) to be weighted count
Given: \((x_1, y_1), \ldots, (x_m, y_m)\) where \(x_i \in X, y_i \in Y = \{-1, +1\}\)

Initialize \(D_1(i) = 1/m\).

For \(t = 1, \ldots, T\):

- Train weak learner using distribution \(D_t\).
- Get weak classifier \(h_t : X \rightarrow \mathbb{R}\).
- Choose \(\alpha_t \in \mathbb{R}\).
- Update:

\[
D_{t+1}(i) = \frac{D_t(i) \exp(-\alpha_t y_i h_t(x_i))}{Z_t}
\]

where \(Z_t\) is a normalization factor

\[
Z_t = \sum_{i=1}^{m} D_t(i) \exp(-\alpha_t y_i h_t(x_i))
\]

Output the final classifier:

\[
H(x) = \text{sign} \left( \sum_{t=1}^{T} \alpha_t h_t(x) \right).
\]

Figure 1: The boosting algorithm AdaBoost.
Boosting: A toy example
Boosting: A toy example

Round 1

\[ h_1 \]

\[ D_2 \]

\[ \varepsilon_1 = 0.30 \]
\[ \alpha_1 = 0.42 \]
Boosting: A toy example

Round 2

\[ \varepsilon_2 = 0.21 \]
\[ \alpha_2 = 0.65 \]
Boosting: A toy example

Thanks, Rob Schapire

Round 3

$\epsilon_3 = 0.14$

$\alpha_3 = 0.92$
Boosting: A toy example

Final Classifier

\[ H_{\text{final}} = \text{sign} \left( \begin{pmatrix} 0.42 & +0.65 & +0.92 \end{pmatrix} \right) \]
What $\alpha_t$ to choose for hypothesis $h_t$?

Training error of final classifier is bounded by:

$$
\frac{1}{m} \sum_{i=1}^{m} \delta(H(x_i) \neq y_i) \leq \frac{1}{m} \sum_{i=1}^{m} \exp(-y_i f(x_i))
$$

Where $f(x) = \sum_{t} \alpha_t h_t(x)$; $H(x) = \text{sign}(f(x))$
What $\alpha_t$ to choose for hypothesis $h_t$?

[Schapire, 1989]

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Where

\[ f(x) = \sum_{t} \alpha_t h_t(x); H(x) = \text{sign}(f(x)) \]

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Where $f(x) = \sum_{t} \alpha_t h_t(x); H(x) = \text{sign}(f(x))$

If we minimize $\prod_{t} Z_t$, we minimize our training error

We can tighten this bound greedily, by choosing $\alpha_t$ and $h_t$ on each iteration to minimize $Z_t$.

$$Z_t = \sum_{i=1}^{m} D_t(i) \exp(-\alpha_t y_i h_t(x_i))$$
What $\alpha_t$ to choose for hypothesis $h_t$?

We can minimize this bound by choosing $\alpha_t$ on each iteration to minimize $Z_t$.

\[
Z_t = \sum_{i=1}^{m} D_t(i) \exp(-\alpha_t y_i h_t(x_i))
\]

Define

\[
\epsilon_t = \sum_{i=1}^{m} D_t(i) \delta(h_t(x_i) \neq y_i)
\]

We can show that:

\[
Z_t = (1 - \epsilon_t) \exp^{-\alpha_t} + \epsilon_t \exp^{\alpha_t}
\]
What $\alpha_t$ to choose for hypothesis $h_t$?

We can minimize this bound by choosing $\alpha_t$ on each iteration to minimize $Z_t$.

$$Z_t = (1 - \varepsilon_t) \exp^{-\alpha_t} + \varepsilon_t \exp^{\alpha_t}$$

For Boolean target function, this is accomplished by [Freund & Schapire ’97]:

$$\alpha_t = \frac{1}{2} \ln \left( \frac{1 - \varepsilon_t}{\varepsilon_t} \right)$$

Where:

$$\varepsilon_t = \sum_{i=1}^{m} D_t(i) \delta(h_t(x_i) \neq y_i)$$
Given: \((x_1, y_1), \ldots, (x_m, y_m)\) where \(x_i \in X, y_i \in Y = \{-1, +1\}\)

Initialize \(D_1(i) = 1/m\).

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\]

\[
\alpha_t = \frac{1}{2} \ln \left( \frac{1 - \epsilon_t}{\epsilon_t} \right)
\]
Strong, weak classifiers

\[ Z_t = \sum_{i=1}^{m} D_t(i) \exp(-\alpha_t y_i h_t(x_i)) \]

- If each classifier is (at least slightly) better than random
  \[ \varepsilon_t < 0.5 \]

- With a few extra steps it can be shown that AdaBoost will achieve zero training error (exponentially fast):

\[
\frac{1}{m} \sum_{i=1}^{m} \delta(H(x_i) \neq y_i) \leq \prod_{t} Z_t \leq \exp \left( -2 \sum_{t=1}^{T} \left( \frac{1}{2} - \varepsilon_t \right)^2 \right)
\]
• Boosting often
  – Robust to overfitting
  – Test set error decreases even after training error is zero

[Schapire, 1989]
Boosting: Experimental Results

Comparison of C4.5, Boosting C4.5, Boosting decision stumps (depth 1 trees), 27 benchmark datasets
AdaBoost and AdaBoost.MH on Train (left) and Test (right) data from Irvine repository. [Schapire and Singer, ML 1999]
Random forest

• A collection of decision trees
• For each tree we select a subset of the attributes (recommended square root of \(|A|\)) and build tree using just these attributes
• An input sample is classified using majority voting
What you need to know about Boosting

• Combine weak classifiers to obtain very strong classifier
  – Weak classifier – slightly better than random on training data
  – Resulting very strong classifier – can eventually provide zero training error

• AdaBoost algorithm

• Most popular application of Boosting:
  – Boosted decision stumps!
  – Very simple to implement, very effective classifier
Boosting and Logistic Regression

Logistic regression assumes:

\[ P(Y = 1|X) = \frac{1}{1 + \exp(f(x))} \]

And tries to maximize data likelihood:

\[ P(D|H) = \prod_{i=1}^{m} \frac{1}{1 + \exp(-y_i f(x_i))} \]

Equivalent to minimizing log loss

\[ \sum_{i=1}^{m} \ln(1 + \exp(-y_i f(x_i))) \]
Boosting and Logistic Regression

Logistic regression equivalent to minimizing log loss

$$\sum_{i=1}^{m} \ln(1 + \exp(-y_if(x_i)))$$

Boosting minimizes similar loss function!!

$$\frac{1}{m} \sum_{i} \exp(-y_if(x_i)) = \prod_{t} Z_t$$

Both smooth approximations of 0/1 loss!
Logistic regression and Boosting

Logistic regression:

- Minimize loss fn
  \[ \sum_{i=1}^{m} \ln(1 + \exp(-y_i f(x_i))) \]
- Define
  \[ f(x) = \sum_{j} w_j x_j \]
  where \( x_j \) predefined

Boosting:

- Minimize loss fn
  \[ \sum_{i=1}^{m} \exp(-y_i f(x_i)) \]
- Define
  \[ f(x) = \sum_{t} \alpha_t h_t(x) \]
  where \( h_t(x_i) \) defined dynamically to fit data
  (not a linear classifier)
- Weights \( \alpha_j \) learned incrementally