Machine learning

Ensemble methods

Corso di Laurea Magistrale in Informatica

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Ensemble methods

Improve performance by combining multiple models, in some way, instead of using a single model.

- train a *committee* of L different models and make predictions by averaging the predictions made by each model on dataset samplings (bagging)
- train different models in sequence: the error function used to train a model depend on the performance of previous models (boosting)

Bagging

- Classifiers (especially some of them, such as decision trees) may have low performances due to their high variance: their behavior may largely differ in presence of slightly different training sets (or even of the same training set).
- For example, in trees, the separations made by splits are enforced at all lower levels: hence, if the data is perturbed slightly, the new tree can have a considerably different sequence of splits, leading to a different classification rule

Bootstrap

- The bootstrap is a fundamental resampling tool in statistics. The basic underlying idea is to estimate the true distribution of data $\mathcal{F}$ by the so-called empirical distribution $\hat{\mathcal{F}}$
- Given the training data $(\mathbf{x}_i, t_i)$, $i = 1, \dots, n$, the empirical distribution function $\hat{\mathcal{F}}$ is defined as

$$\hat{p}(\mathbf{x}, t) = \begin{cases} \frac{1}{n} & \text{if } \exists i : (\mathbf{x}, t) = (\mathbf{x}_i, t_i) \\ 0 & \text{otherwise} \end{cases}$$

- This is just a discrete probability distribution, putting equal weight $\frac{1}{n}$ on each of the observed training points

Bootstrap

- A bootstrap sample of size m from the training data is

$$(\mathbf{x}_i^*, t_i^*) \qquad i = 1, \ldots, m$$

  where each $(\mathbf{x}_i^*, t_i^*)$ is drawn uniformly at random from $(\mathbf{x}_1, t_1), \ldots, (\mathbf{x}_n, t_n)$, with replacement
- This corresponds exactly to m independent draws from $\hat{\mathcal{F}}$: it approximates what we would see if we could sample more data from the true $\mathcal{F}$. We often consider $m = n$, which is like sampling an entirely new training set

Bagging

- Given a training set $(\mathbf{x}_i, y_i)$, $i = 1, \dots, n$, bagging averages the predictions done by classifiers of the same type (such as decision trees) over a collection of boostrap samples. For $b = 1, \dots, B$ (e.g., B = 100), n bootstrap items $(\mathbf{x}_i^b, y_i^b)$, $i = 1, \dots, n$ are sampled and a classifier is fit on this set.
- At the end, to classify an input x, we simply take the most commonly predicted class, among all B classifiers
- This is just choosing the class with the most votes
- In the case of regression, the predicted value is derived as the average among the predictions returned by the B regressors

Bagging variant

If the used classifier returns class probabilities $\hat{p}_k^b(\mathbf{x})$, the final bagged probabilities can be computed by averaging

$$p_k^b(\mathbf{x}) = \frac{1}{B}\sum_{b=1}^{B}\hat{p}_k^b(\mathbf{x})$$

the predicted class is, again, the one with highest probability

Bagging classification

- Why is bagging working?
- Let us consider, for simplicity, a binary classification problem. Suppose that for a given input $\mathbf{x}$, we have B independent classifiers, each with a given misclassification rate e (for example, $e = 0.4$). Assume w.l.o.g. that the true class at $\mathbf{x}$ is 1: so the probability that the b-th classifier predicts class 0 is $e = 0.4$
- Let $B_0 \leq B$ be the number of classifiers returning class 0 on input $\mathbf{x}$: the probability of B_0 is clearly distributed according to a binomial (if classifiers are independent)

$$B_0 \sim \text{Binomial}(B, e)$$

the misclassification rate of the bagged classifier is then

$$p\left(B_0 > \frac{B}{2}\right) = \sum_{k=\frac{B}{2}+1}^{B} \binom{B}{k} e^k (1-e)^{B-k}$$

which tends to 0 as B increases.

Bagging regression

- Expected error of one model $y_i(\mathbf{x})$ wrt the true function $h(\mathbf{x})$:

$$E_{\mathbf{x}}[(y_i(\mathbf{x}) - h(\mathbf{x}))^2] = E_{\mathbf{x}}[\varepsilon_i(\mathbf{x})^2]$$

- Average expected error of the models

$$E_{av} = \frac{1}{m}\sum_{i=1}^{m} E_{\mathbf{x}}[\varepsilon_i(\mathbf{x})^2]$$

- Committee expected error

$$E_c = E_{\mathbf{x}}\left[\left(\frac{1}{m}\sum_{i=1}^{m} y_i(\mathbf{x}) - h(\mathbf{x})\right)^2\right] = E_{\mathbf{x}}\left[\left(\frac{1}{m}\sum_{i=1}^{m} \varepsilon_i(\mathbf{x})\right)^2\right]$$

  If $E_{\mathbf{x}}[\varepsilon_i(\mathbf{x})\varepsilon_j(\mathbf{x})] = 0$ if $i \neq j$ (errors are uncorrelated) then $E_c = \frac{1}{m}E_{av}$.
- This is usually not verified: errors from different models are highly correlated.

Random forest

Application of bagging to a set of (random) decision trees: classification performed by voting.

1. For $b = 1$ to B:
   1.1 Bootstrap sample from training set
   1.2 Grow a decision tree T_b on such data by performing the following operations for each node:
      1.2.1 select m variables at random
      1.2.2 pick the best variable among them
      1.2.3 split the node into two children
2. output the collection of trees $T_1, \ldots, T_B$

Overall prediction is performed as majority (for classification) or average (for regression) among trees predictions.

Boosting

- Boosting is a procedure to combine the output of many weak classifiers to produce a powerful committee.
- A weak classifier is one whose error rate is only slightly better than random guessing.
- Boosting produces a sequence of weak classifiers $y_m(x)$ for $m = 1, \dots, m$ whose predictions are then combined through a weighted majority to produce the final prediction

$$y(\mathbf{x}) = \mathrm{sgn}\left(\sum_{j=1}^{m} \alpha_j y_j(\mathbf{x})\right)$$

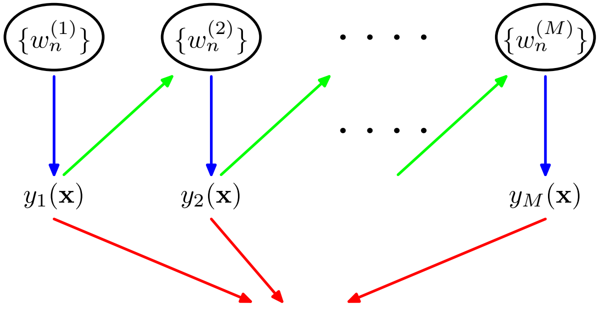
- Each $\alpha_j > 0$ is computed by the boosting algorithm and reflects how accurately y_m classified the data.

Boosting

Adaboost (adaptive boosting)

- Models are trained in sequence: each model is trained using a weighted form of the dataset
- Element weights depend on the performances of the previous models (misclassified points receive larger weights)
- Predictions are performed through a weighted majority voting scheme on all models

Boosting



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

Adaboost

Binary classification, dataset $(\mathbf{X}, \mathbf{t})$ of size n, with $t_i \in \{-1, 1\}$. The algorithm maintains a set of weights $w(\mathbf{x}) = (w_1, \ldots, w_n)$ associated to the dataset elements.

- Initialize weights as $w_i^{(0)} = \frac{1}{n}$ for $i = 1, \ldots, n$
- For $j = 1, \ldots, m$:
    - Train a weak learner $y_j(\mathbf{x})$ on $\mathbf{X}$ in such a way to minimize the weighted misclassification wrt to $w^{(j)}(\mathbf{x})$.
    - Let

$$\pi^{(j)} = \frac{\sum_{\mathbf{x}_i \in \mathcal{E}^{(j)}} w_i^{(j)}}{\sum_i w_i^{(j)}}$$

  where $\mathcal{E}^{(j)}$ is the set of dataset elements misclassified by $y_j(\mathbf{x})$.

    - If $\pi^{(j)} > \frac{1}{2}$, consider the reverse learner, which returns opposite predictions for all elements.
    - $\pi^{(j)}$ can be interpreted as the probability that a random item from the training set is misclassified, assuming that item $\mathbf{x}_i$ can be sampled with probability $\frac{w_i^{(j)}}{\sum_i w_i^{(j)}}$

Adaboost

- Compute the learner confidence as log odds of a random item being well classified $(1-\pi^{(j)})$ vs being misclassified $\pi^{(j)}$

$$\alpha_j = \frac{1}{2}\log\frac{1-\pi^{(j)}}{\pi^{(j)}} > 0$$

- For each $\mathbf{x}_i$, update the corresponding weight as follows

$$w_i^{(j+1)} = w_i^{(j)} e^{-\alpha_j t_i y_j(\mathbf{x}_i)}$$

which results into

$$w_i^{(j+1)} = \begin{cases} w_i^{(j)} e^{\alpha_j} > w_i^{(j)} & \text{if } \mathbf{x}_i \in \mathcal{E}^{(j)} \\ w_i^{(j)} e^{-\alpha_j} < w_i^{(j)} & \text{otherwise} \end{cases}$$

- Normalize the set of $w_i^{(j+1)}$ by dividing each of them by $\sum_{i=1}^n w_i^{(j+1)}$, in order to get a distribution

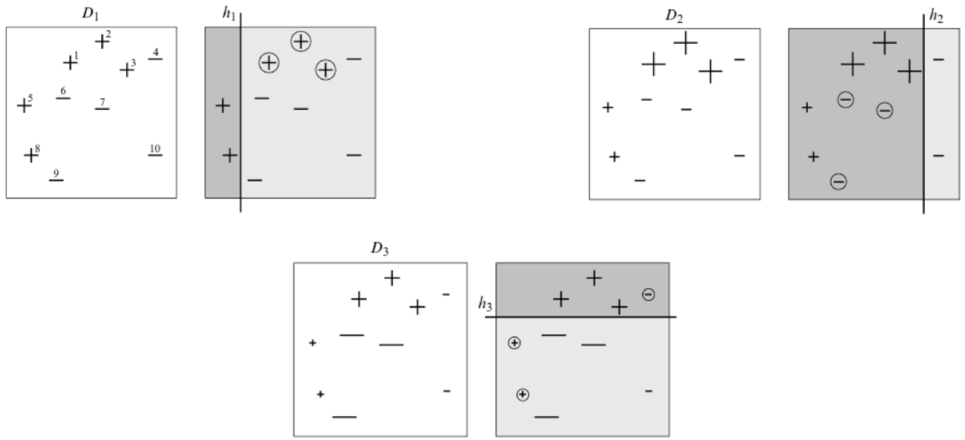
Adaboost

The overall prediction is

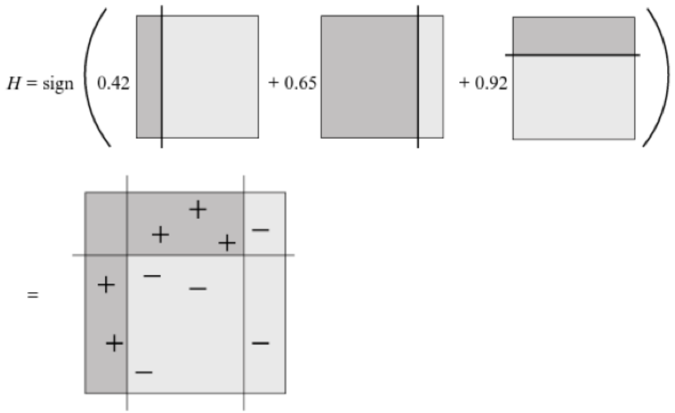
$$y(\mathbf{x}) = \text{sgn}\left(\sum_{j=1}^{m} \alpha_j y_j(\mathbf{x})\right)$$

since $y_j(\mathbf{x}) \in \{-1, 1\}$, this corresponds to a voting procedure, where each learner vote (class prediction) is weighted by the learner confidence.

AdaBoost



ADABOOST



Why does it work?

- It minimizes a loss function related to classification error
- Suppose we have a classifier $y(\mathbf{x}) = \text{sgn}\, f(\mathbf{x})$
- We know that 0/1 loss

$$l(y(\mathbf{x}), t) = \begin{cases} 0 & \text{if } tf(\mathbf{x}) > 0 \\ 1 & \text{otherwise} \end{cases}$$

  has drawbacks (non convex, gradient 0 almost everywhere). We need a surrogate loss.
- Exponential loss

$$l(y(\mathbf{x}), t) = e^{-tf(\mathbf{x})}$$

Additive models

- Additive models are defined as the additive composition of simple “base” predictors

$$y(\mathbf{x}) = \sum_{j=1}^{m} \alpha_j \overline{y}_j(\mathbf{x})$$

  where, for each j, α_j is a weight and $\overline{y}_j(\mathbf{x}) = h(\mathbf{x}; \mathbf{w}_j) \in \mathbb{R}$ is a simple function of the input $\mathbf{x}$ parameterized by $\mathbf{w}_j \in \mathbb{R}^p$ for a given p
- in this case, the predictors are binary classifiers; that is, $\overline{y}_j(\mathbf{x}) = h(\mathbf{x}; \mathbf{w}_j) \in \{-1, 1\}$

Fitting additive models

- As usual, an additive model is fit by minimizing a loss function averaged over the training data:

$$\min_{\boldsymbol{\alpha},\mathbf{W}} L\left(t_i, y(\mathbf{x})\right) = \min_{\boldsymbol{\alpha},\mathbf{W}} \sum_{i=1}^{n} L\left(t_i, \sum_{k=1}^{m} \alpha_k h(\mathbf{x}_i; \mathbf{w}_k)\right)$$

  with $\boldsymbol{\alpha} = \{\alpha_1, \ldots, \alpha_m\}$ and $\mathbf{W} = \cup_{j=1}^{m} \mathbf{w}_j$
- For many loss functions L and/or additive predictors h this is too hard

Forward stagewise additive modeling

We may make things simpler by greedily adding one predictor at a time as follows.

- Set $y_0(\mathbf{x}) = 0$
- For $k = 1, \ldots, m$:
    - Compute

$$(\hat{\alpha}_k, \hat{\mathbf{w}}_k) = \underset{\alpha_k, \mathbf{w}_k}{\operatorname{argmin}} \sum_{i=1}^{n} L\left(t_i, y_{k-1}(\mathbf{x}_i) + \alpha_k h(\mathbf{x}_i; \mathbf{w}_k)\right)$$

    - Set $y_k(\mathbf{x}) = y_{k-1}(\mathbf{x}) + \hat{\alpha}_k h(\mathbf{x}; \hat{\mathbf{w}}_k)$

That is, fitting is performed not modifying previously added terms (greedy paradigm)

Adaboost as additive model

Adaboost can be interpreted as fitting an additive model with exponential loss

$$L(t, y(\mathbf{x})) = e^{-ty(\mathbf{x})}$$

that is, minimizing

$$\sum_{i=1}^{n} e^{-t_i \sum_{k=1}^{m} \alpha_k h(\mathbf{x}_i;\mathbf{w}_k)}$$

with respect to $\mathbf{w}_1, \ldots, \mathbf{w}_m$ and $\alpha_1, \ldots, \alpha_m$.

In Adaboost, we have that $p = n$. That is, the number of parameters in $h(\mathbf{x}, \mathbf{w})$ is equal to the number of items: hence, $\mathbf{w}_k = (w_{k1}, \ldots, w_{kn})$ for all k.

Gradient boosting

General idea:

- Fit an additive model $\sum_{j=1}^{m} \alpha_j y_j(\mathbf{x})$ in a forward stage-wise manner.
- At each stage, introduce a weak learner to compensate the shortcomings of existing ones.
- Shortcomings are identified by high-weight data points.

Gradient boosting

- You are given $(\mathbf{x}_i, t_i)$, $i = 1, \ldots, n$, and the task is to fit a model $y(\mathbf{x})$ to minimize square loss.
- Assume a model $y^{(1)}(\mathbf{x})$ is available, with residuals $t_i - y_i^{(1)} = t_i - y^{(1)}(\mathbf{x}_i)$
- A new dataset $(\mathbf{x}_i, t_i - y_i^{(1)})$, $i = 1, \ldots, n$ can be defined, and a model $h^{(1)}(\mathbf{x})$ can be fit to minimize square loss wrt such dataset
- Clearly, $y_2(\mathbf{x}) = y_1(\mathbf{x}) + h_1(\mathbf{x})$ is a model which improves $y_1(\mathbf{x})$
- The role of $h_1(\mathbf{x})$ is to compensate the shortcoming of $y(\mathbf{x})$
- If $y_2(\mathbf{x})$ is unsatisfactory, we may define new models $h_2(\mathbf{x})$ and $y_3(\mathbf{x}) = y_2(\mathbf{x}) + h_2(\mathbf{x})$

Gradient boosting

How is this related to gradient descent?

- Let us consider the squared loss function $L(t, y) = \frac{1}{2}(t - y)^2$
- We want to minimize the empirical risk $R = \sum_{i=1}^{n} L(t_i, y_i)$ by adjusting $y_1, \ldots, y_n$, considered as parameters
- For each y_i we consider the derivative

$$\frac{\partial R}{\partial y_i} = y_i - t_i$$

  The residuals correspond then to negative gradients

$$t_i - y_i = -\frac{\partial R}{\partial y_i}$$

- Model $h(\mathbf{x})$ can then be derived by considering the dataset

$$(\mathbf{x}_i, t_i - y_i) = \left(\mathbf{x}_i, -\frac{\partial R}{\partial y_i}\right) \qquad i = 1, \ldots, n$$

Gradient boosting

Looking at the new dataset

$$\left\{\left(\mathbf{x}_i, -\frac{\partial R}{\partial y_i}\right), \ldots, \left(\mathbf{x}_n, -\frac{\partial R}{\partial y_n}\right)\right\}$$

We wonder what is the meaning of looking for a predictor h which fits such points.

- The idea is that $h(\mathbf{x}_i)$ should be small if the current cost derived from the current prediction y_i of $\mathbf{x}_i$ is almost constant: modifying the prediction results into a limited gain wrt the cost
- similarly, if the cost would increase considerably by increasing the prediction value, then $h(\mathbf{x}_i)$ should modify such cost by decreasing it; that is it should be more negative
- finally, by symmetry, if the cost would decrease considerably by increasing the prediction value, then $h(\mathbf{x}_i)$ should modify such cost by increasing it; that is it should be more positive

Gradient boosting for regression

The following algorithm results

- Set $y^{(1)}(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^{n} t_i$
- For $k = 1, \ldots, m$:
    - Compute negative gradients

$$-g_i^{(k)} = -\frac{\partial R}{\partial y_i}\bigg|_{y_i=y^{(k)}(\mathbf{x}_i)} = -\frac{\partial}{\partial y_i}L(t_i, y_i)\bigg|_{y_i=y^{(k)}(\mathbf{x}_i)} = t_i - y^{(k)}(\mathbf{x}_i)$$

    - Fit a weak learner $h^{(k)}(\mathbf{x})$ to negative gradients, considering dataset $(\mathbf{x}_i, -g_i^{(k)})$, $i = 1, \ldots, n$
    - Derive the new classifier $y^{(k+1)}(\mathbf{x}) = y^{(k)}(\mathbf{x}) + h^{(k)}(\mathbf{x})$

Gradient boosting for regression

- The benefit of formulating this algorithm using gradients is that it allows us to consider other loss functions and derive the corresponding algorithms in the same way.
- For example, square loss is easy to deal with mathematically, but not robust to outliers, i.e. pays too much attention to outliers.
- Different loss functions
    - Absolute loss
        - $$L(t, y) = |t - y|$$
        - $$-g = \text{sgn}(t - y)$$
    - Huber loss
        - $$L(t, y) = \begin{cases} \frac{1}{2}(t - y)^2 & |t - y| \leq \delta \\ \delta(|t - y|) - \frac{\delta}{2} & |t - y| > \delta \end{cases}$$
        - $$-g = \begin{cases} y - t & |t - y| \leq \delta \\ \delta \cdot \text{sgn}(t - y) & |t - y| > \delta \end{cases}$$

Gradient boosting for classification

A similar approach can be applied on K-class classification, with

$$R = \sum_{i=1}^{n} L(t_i, y_1(\mathbf{x}_i), \ldots, y_K(\mathbf{x}_i)) = \sum_{i=1}^{n} L((t_{i1}, \ldots, t_{iK}), (y_{i1}, \ldots, y_{iK}))$$

for a given loss function

Which weak learners?

- Regression trees (special case of decision trees)
- Decision stumps (trees with only one node)