Machine Learning

Ensemble Methods: Boosting

FAST

DISCOVERING THE FUTURE

Topics of previous lectures

- ✓ Ingredients of Machine Learning
- ✓ Classification Basics, Basic Linear Classifier
- ✓ K-Nearest Neighbours and Naive Bayes Classifier
- ✓ Linear and Quadratic Discriminant Analysis
- ✓ Support Vector Machines (SVM)
- ✓ Decision Trees
- ✓ Ensemble Methods (Bagging, Weighted Voting, Stacking)
- ✓ Regression Methods
- ✓ Evaluation and Scoring of Classifiers

Topics of today's lecture

- Boosting
- AdaBoost
- Gradient Boosting

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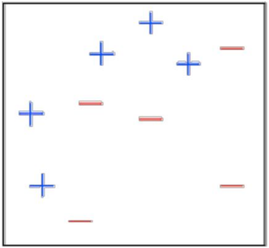
- No!
- The idea of boosting is that each model corrects the mistakes of the previous models in the ensemble.

Intuition behind AdaBoost

The idea of **Boosting** is that each model corrects the weaknesses (mistakes) of the previous models in the ensemble.



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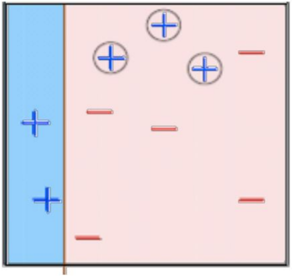

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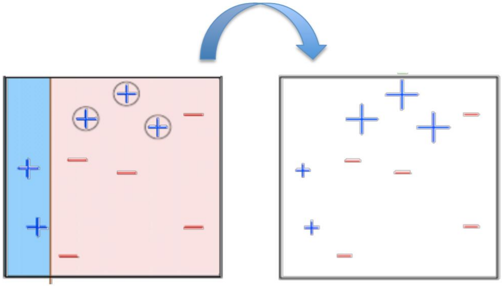

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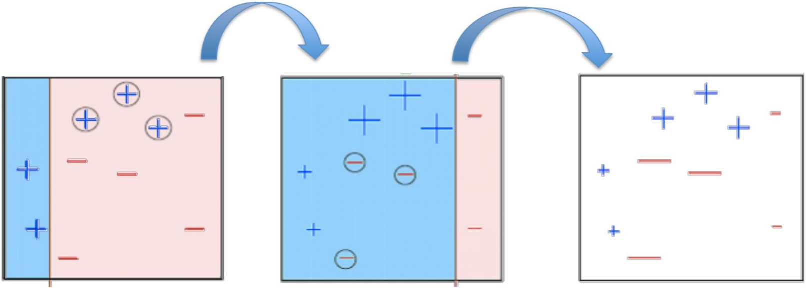

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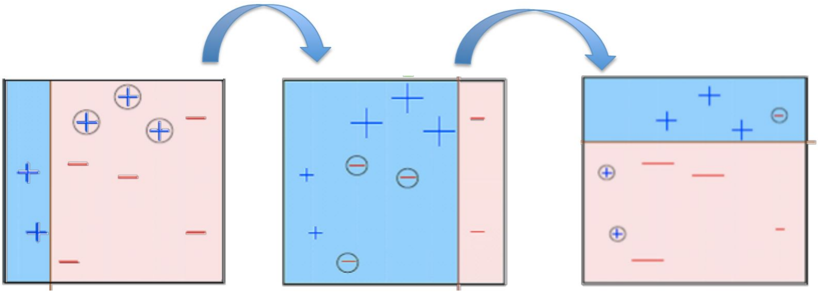

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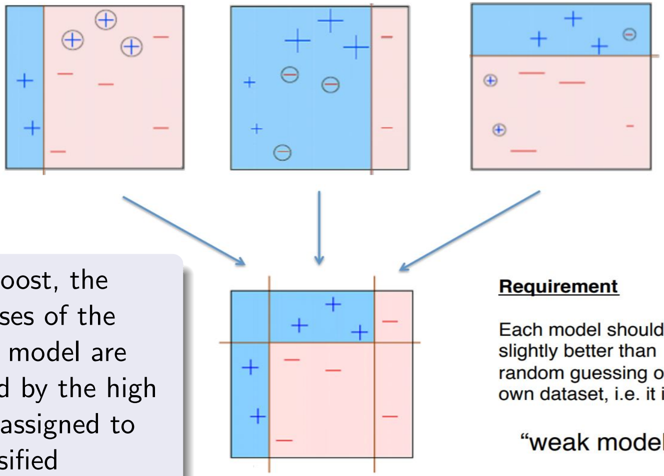

In AdaBoost, the weaknesses of the previous model are identified by the high weights assigned to missclassified instances.

Requirement

Each model should be slightly better than random guessing on its own dataset, i.e. it is a...

"weak model"

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- Create a weighted dataset, where the first model would have 50% accuracy
- Then the second model is forced to do better than the first one
- Repeat the same with successive models

AdaBoost (Freund and Schapire 1995)

Suppose that the labels are encoded as ± 1.

Algorithm AdaBoost($D, T, \mathscr{A}$) – train an ensemble of binary classifiers from reweighted training sets.

Input : training data set D; ensemble size T; learning algorithm $\mathscr{A}$.
Output : weighted ensemble of models.

```
w_{1i} ← 1/|D| for all x_i ∈ D ;                      // start with uniform weights
for t = 1 to T do
    run 𝒜 on D with weights w_{ti} to produce a model h_t;
    calculate weighted error ε_t = Σ_{i=1}^{|D|} w_{ti} I[h_t(x_i) ≠ y_i];
    if ε_t ≥ 1/2 then
        set T ← t − 1 and break
    end
    α_t ← (1/2) ln((1−ε_t)/ε_t) ;                      // confidence for this model
    w_{(t+1)i} ← w_{ti} e^{−α_t y_i h_t(x_i)} for i = 1,…,|D| ;          // update weights
    w_{(t+1)i} ← w_{(t+1)i} / Σ_{j=1}^{|D|} w_{(t+1)j} for i = 1,…,|D| ;   // renormalize weights
end
return H(x) = Σ_{t=1}^{T} α_t h_t(x)
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  if $\epsilon_t \geq 1/2$ **then**
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end
return $H(\mathbf{x}) = \sum_{t=1}^{T} \alpha_t h_t(\mathbf{x})$

On a test instance AdaBoost predicts: $\hat{y} = sign(H(\mathbf{x})) = sign(\sum_{t=1}^{T} \alpha_t h_t(\mathbf{x}))$

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Here the only part of the equation depending on h_t is the second sum and L is minimized if we choose h_t s.t. $\sum_{y_i \neq h_t(\mathbf{x}_i)} w_i^{(t)}$ is minimized (assuming $\alpha_t > 0$), that is the classifier with the lowest weighted error.

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Now let's derive the weight α_t that minimizes the loss function.

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since the weighted error of the weak classifier is $\epsilon_t = \frac{\sum_{y_i \neq h_t(\mathbf{x}_i)} w_i^{(t)}}{\sum_{i=1}^{N} w_i^{(t)}}$,

then $\alpha_t = \frac{1}{2}\log\left(\frac{1-\epsilon_t}{\epsilon_t}\right)$

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- This ensures that the current ensemble would have weighted error 50%
- As weak learner is expected to achieve less than 50% weighted error, it is also expected to learn something new (that the ensemble does not "know" yet)

AdaBoost for regression (AdaBoost.R2 (Drucker, 1997))

Input : training data set D; ensemble size T ; learning algorithm A
Output : weighted ensemble of models

1. Start with uniform weights $w_i^{(1)} = 1/|D| \, \forall \mathbf{x}_i \in D$

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      let $Z_t = \max_{j \in \{1, \ldots, |D|\}} |y_j - h_t(x_j)|$

      $e_i^{(t)} = \frac{|y_i - h_t(x_i)|}{Z_t}$

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   7. Update the weights $w_i^{(t+1)} = w_i^{(t)} \beta_t^{1-e_i^{(t)}}$

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      $\epsilon_t = \sum_{i=1}^{|D|} w_i^{(t)} e_i^{(t)}$
   5. If $\epsilon_t \geq \frac{1}{2}$ then set $t = T - 1$ and break
   6. Let $\beta_t = \frac{\epsilon_t}{1-\epsilon_t}$
   7. Update the weights $w_i^{(t+1)} = w_i^{(t)} \beta_t^{1-e_i^{(t)}}$
   8. Normalize the weights $w_i^{(t+1)} = \frac{w_i^{(t+1)}}{\sum_{i=1}^{|D|} w_i^{(t+1)}}$

AdaBoost for regression (AdaBoost.R2 (Drucker, 1997))

Input : training data set D; ensemble size T ; learning algorithm A

Output : weighted ensemble of models

1 Start with uniform weights $w_i^{(1)} = 1/|D| \, \forall \mathbf{x}_i \in D$

2 For $t = 1, \ldots, T$ do

 3 Run A on D with weights $w_i^{(t)}$ to produce a model h_t ;

 4 Calculate weighted error

 let $Z_t = \max_{j \in \{1,\ldots,|D|\}} |y_j - h_t(x_j)|$

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 8 Normalize the weights $w_i^{(t+1)} = \frac{w_i^{(t+1)}}{\sum_{i=1}^{|D|} w_i^{(t+1)}}$

9 Return the weighted median of $h_t(x)$ for $t = 1, \ldots, T$, using $\ln(\frac{1}{\beta_t})$ as weights

AdaBoost.R2

The errors in step 4 are usually calculated using the following loss functions

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- How would you improve the performance of the initial model?

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You want to improve the model such that

$$\hat{f}(x_1) + h(x_1) = y_1$$
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We can fit a regression tree to data
$(x_1, y_1 - F(x_1)), (x_2, y_2 - F(x_2)), \dots, (x_n, y_n - F(x_n))$

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- In this way we can improve the predictions from individual models

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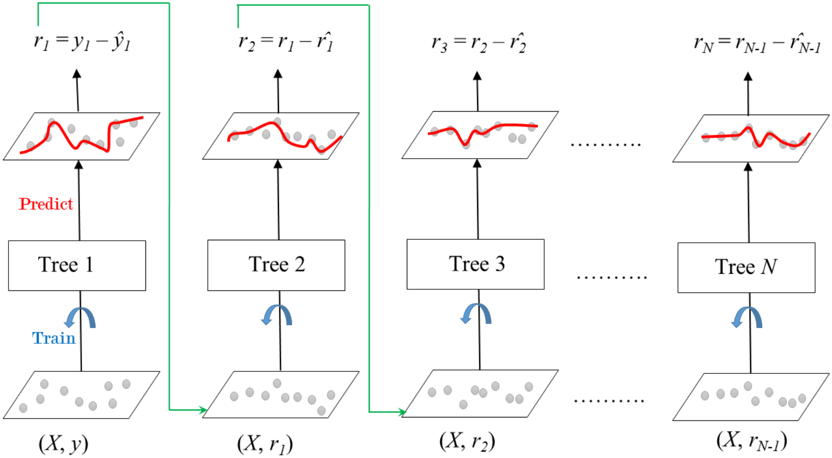
- The residuals are the negative gradients

$$y_i - \hat{f}(x_i) = -\frac{\partial J}{\partial \hat{f}(x_i)}$$

Gradient Boosting



Gradient Boosting for Regression (with squared loss)

Input : training data set $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$; ensemble size M, loss function $L(y, f(x)) = (y - f(x))^2$, learning rate α

Output : ensemble of models

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> The learning rate for each update may also be optimized inside the algorithm

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- The probability $\mathbb{P}(Y_i = k|X = \mathbf{x}_i)$ is modeled as a softmax of the final outcomes of the K functions

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Input : training data set $\{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^n$ (1-hot encoded $\mathbf{y}$); ensemble size M, loss function $L(y, f(x)) = -\sum_{j=1}^K y_j \log(f^{(j)}(x))$, learning rate α
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Gradient Boosting for Classification

Input : training data set $\{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^n$ (1-hot encoded $\mathbf{y}$); ensemble size M, loss function $L(y, f(x)) = -\sum_{j=1}^K y_j \log(f^{(j)}(x))$, learning rate α
Output : ensemble of models

1. Initialize the models with prior probability values $\hat{f}^{(j)}(x) = \frac{1}{n}\sum_{i=1}^n \mathbf{y}_i$ for $j = 1, \dots, K$
2. For $m = 1, \dots, M$ do
    1. Compute the **pseudo-residuals**:

    $$r_{im}^{(j)} = -\Big(\frac{\partial L(y_i, \hat{f}(x_i))}{\partial \hat{f}^{(j)}(x_i)}\Big),\ i = 1, \dots, n,\ j = 1, \dots, K$$

    2. Fit K **regression** models (typically a weak learner) $h_m^{(j)}(x)$ to pseudo-residuals $\{(\mathbf{x}_i, r_{im}^{(j)})\}_{i=1}^n$

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    3. Update the models: $\hat{f}_m^{(j)} = \hat{f}_{m-1}^{(j)}(x) + \alpha h_m^{(j)}(x)$

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    4. Apply softmax function to obtain probabilities $\hat{f}_m^{(j)} = \frac{\exp(\hat{f}_m^{(j)})}{\sum_{j=1}^{K} \exp(\hat{f}_m^{(j)})}$

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3. Return $\hat{f}_M(x)$. Predict the label with the highest probability.

What have we learned today?

- ✓ Boosting
- ✓ AdaBoost
- ✓ Gradient Boosting