Ensemble learning

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Ensemble learning

Definition 1

Ensemble learning - using multiple machine learning methods for a given problem and integrating their output to obtain final result.

Synonyms: committee-based learning, multiple classifier systems. Closely relates to **data fusion** - integration of multiple data representing the same real-world object into useful representation.

Applications:

- supervised methods: regression, classification
- unsupervised methods: clustering

Motivation of ensembles

- Benefits for prediction:
  - increased accuracy
  - increased robustness.
- Justification: some predictors are compensating the errors of other predictors
- When to use:
  - existing model hypothesis space is too narrow to explain the true one
  - too small dataset to figure out concretely the exact model hypothesis
  - avoid local optima of optimization methods
- Frequently the task itself promotes usage of ensembles (such as computer security):
  - multiple sources of diverse information
  - different abstraction levels need to be united

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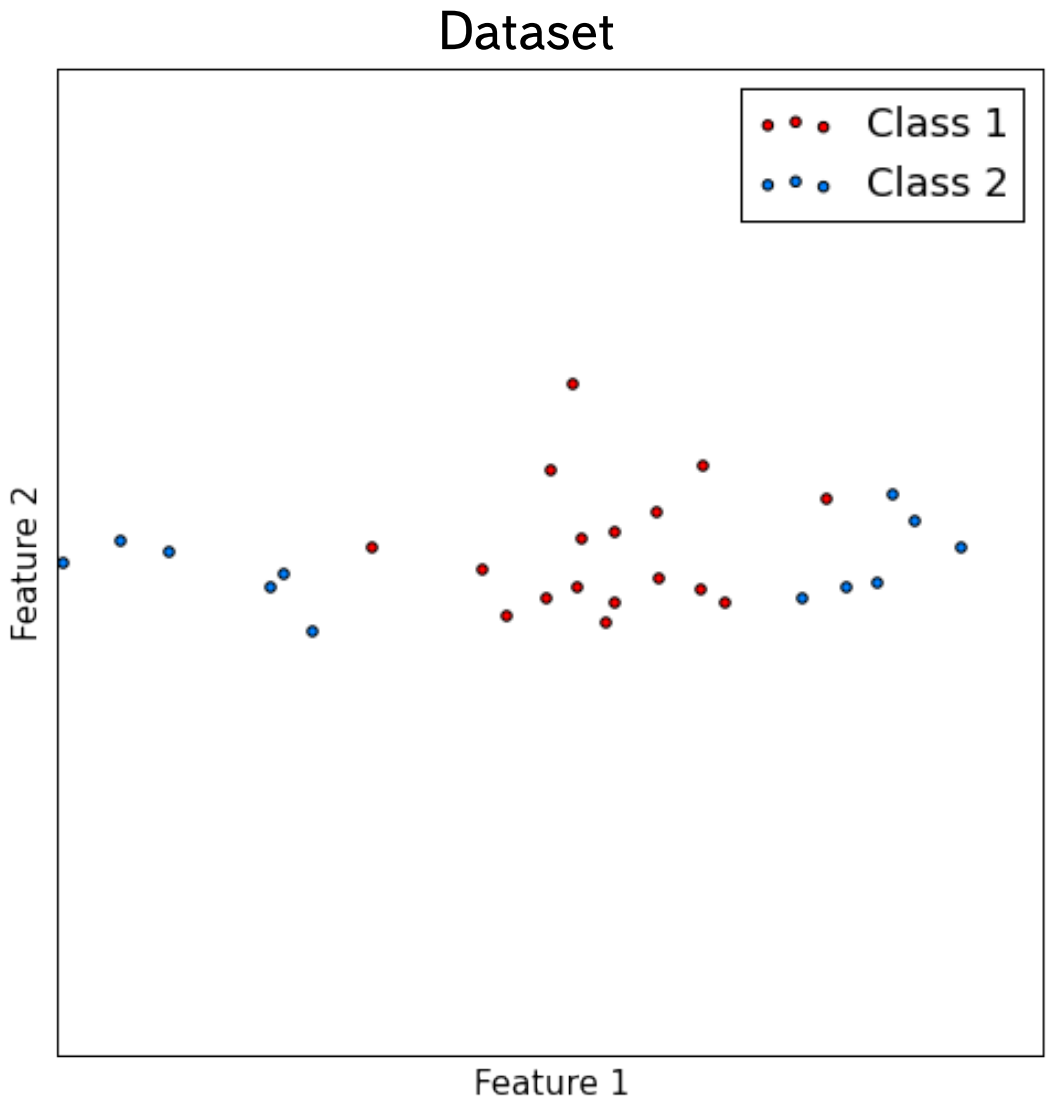
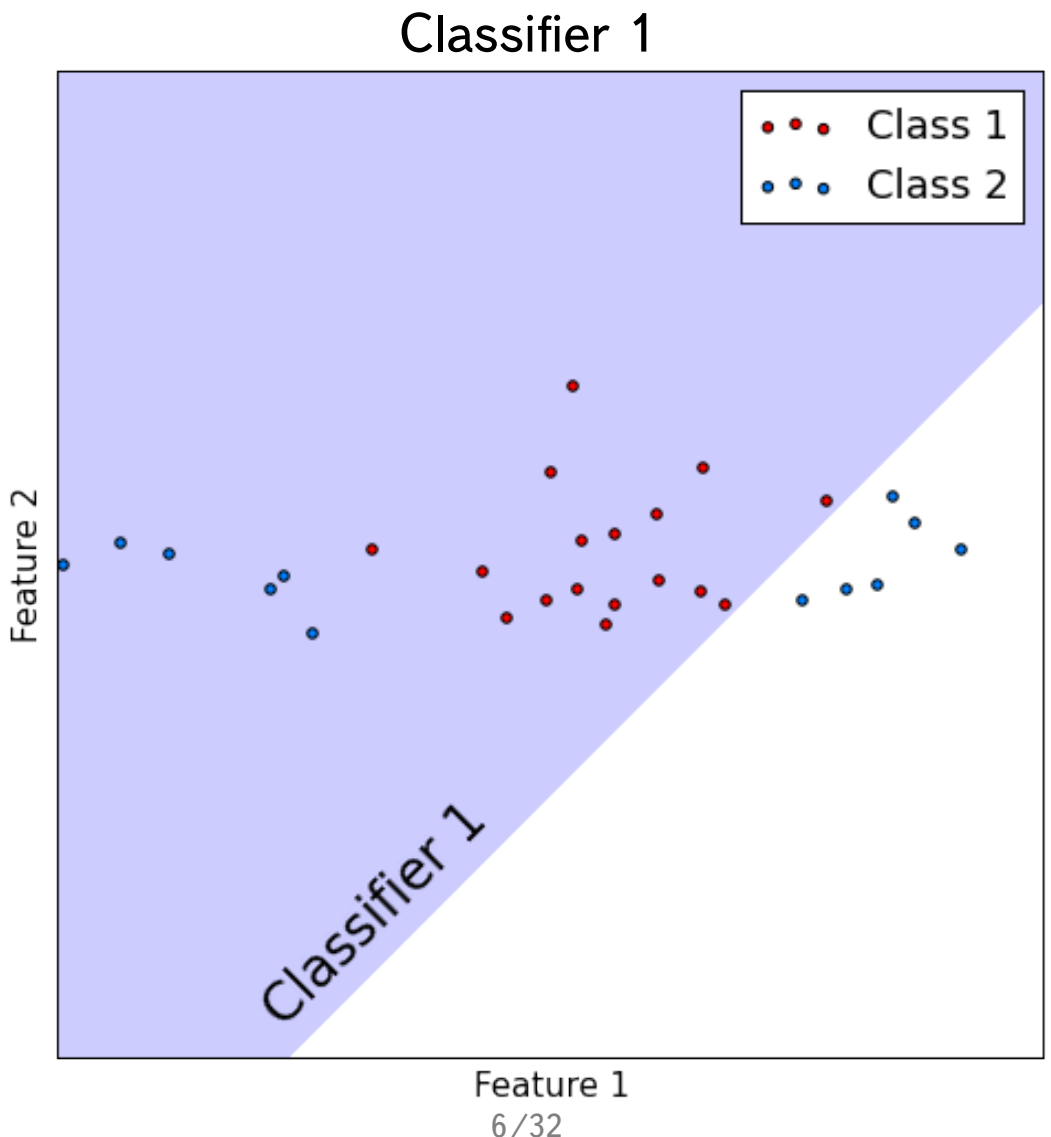
Motivation for classification



Motivation for classification



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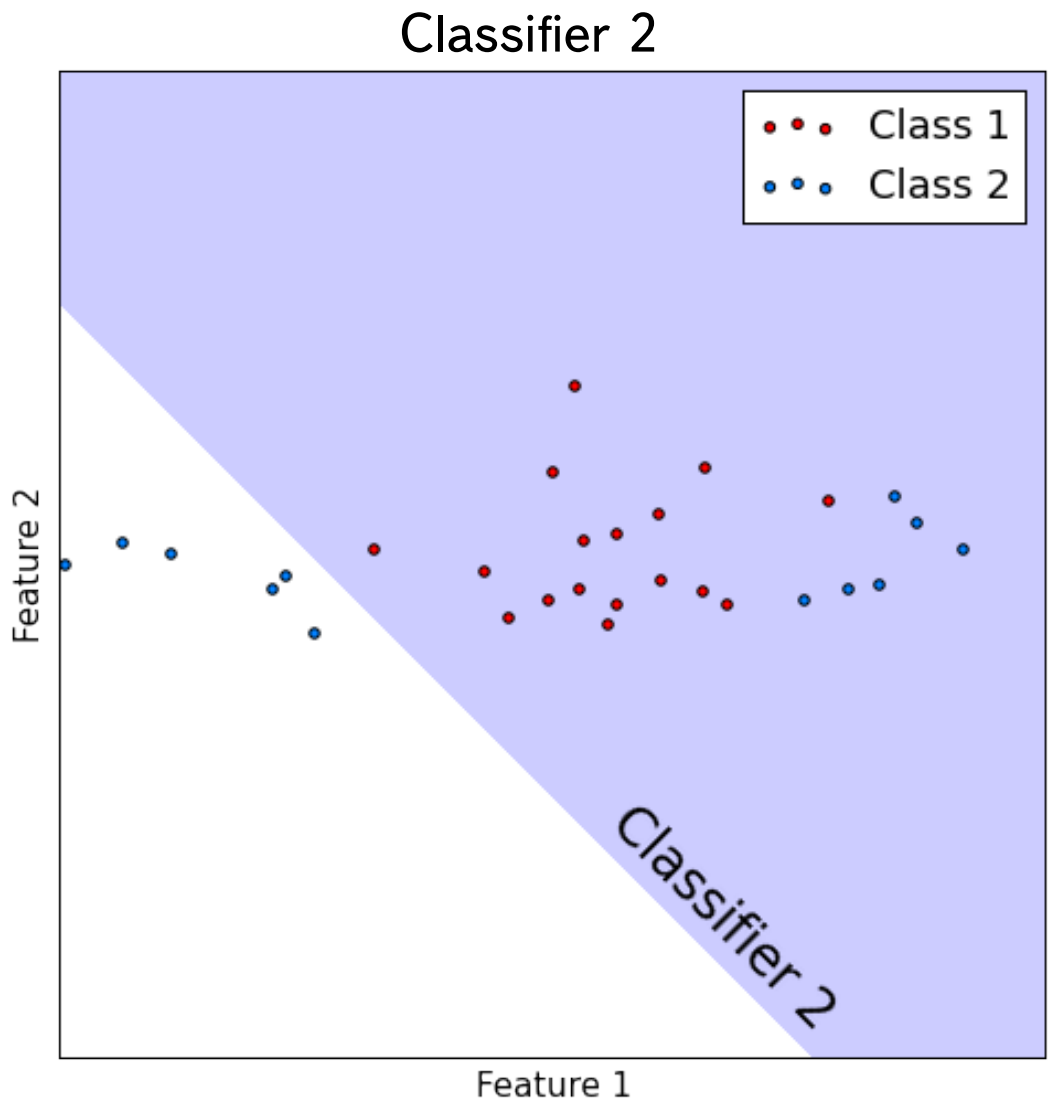
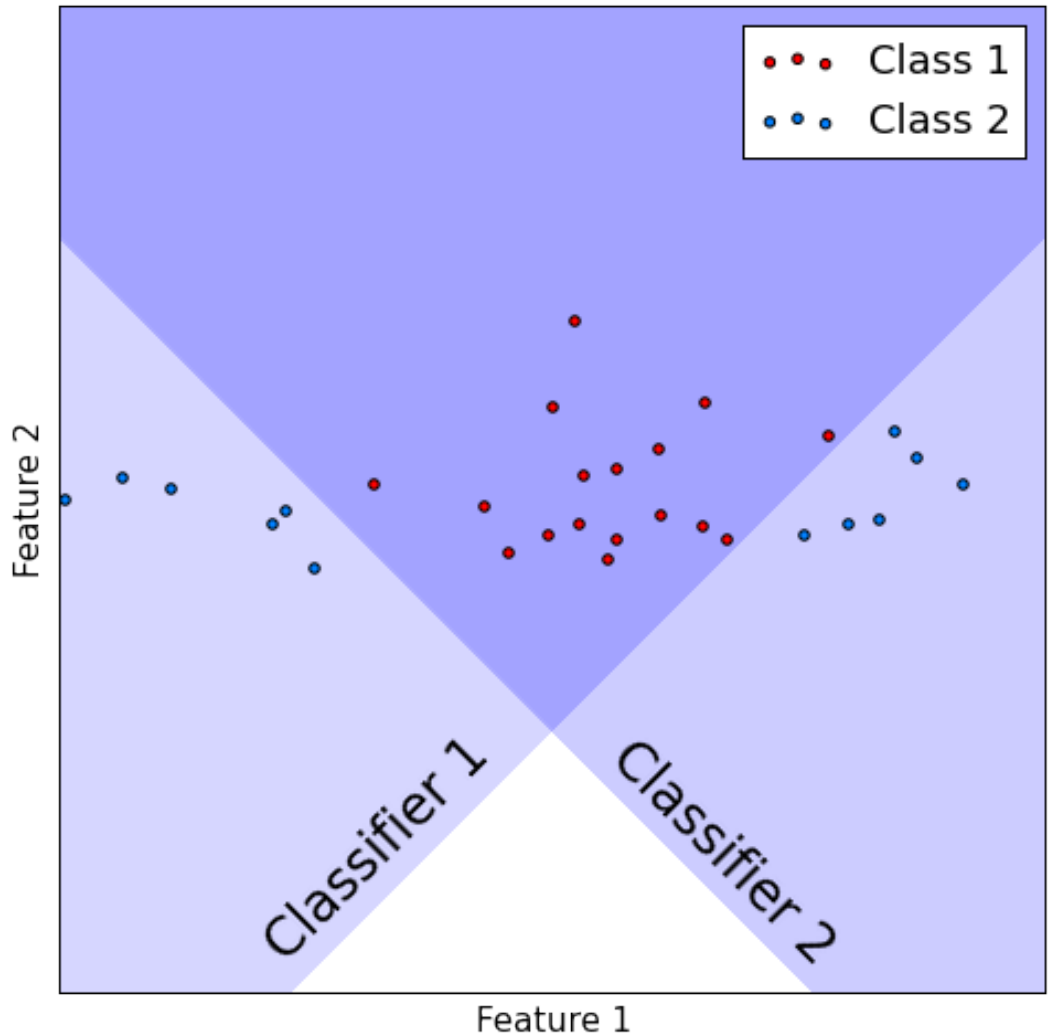
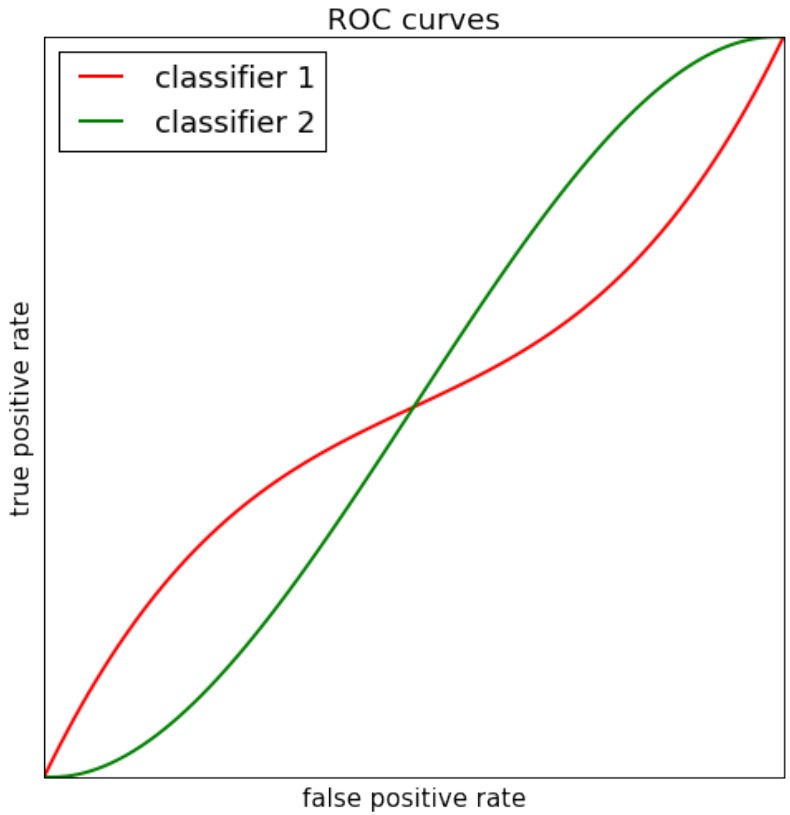


Motivation for classification

Classifier 1 and classifier 2 combined using AND rule

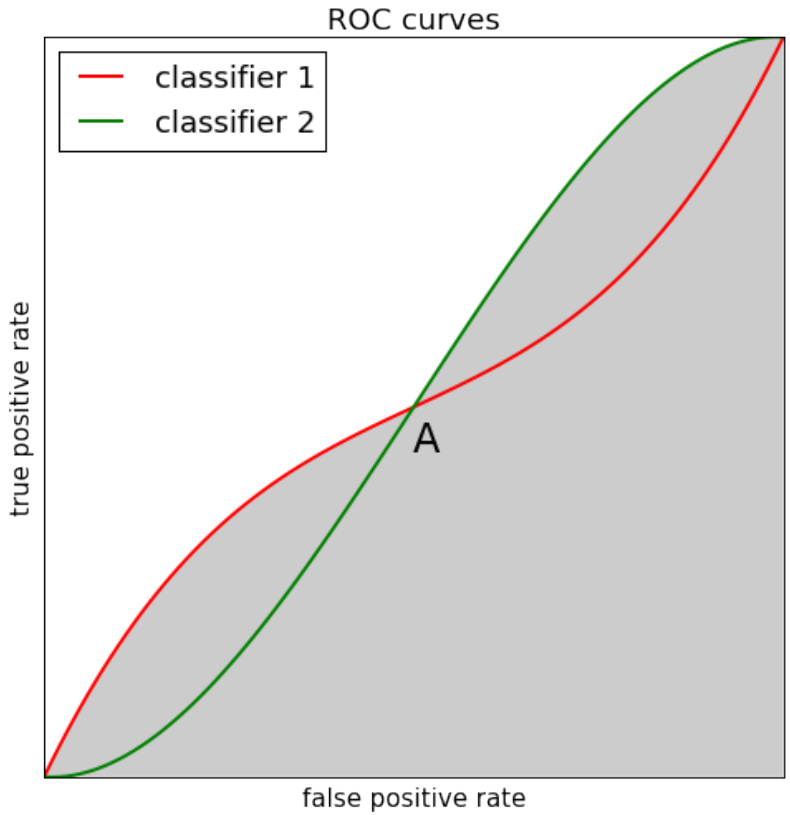


ROC curve of classifier combination



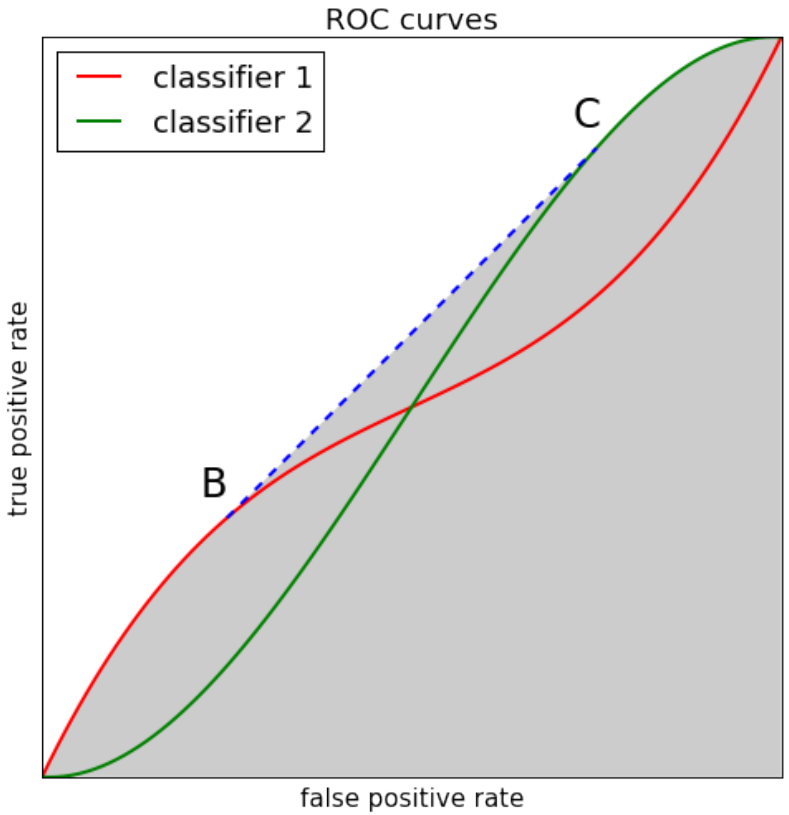
Suppose we have two classifiers and want to optimize AUC of their combination.

ROC curve of classifier combination



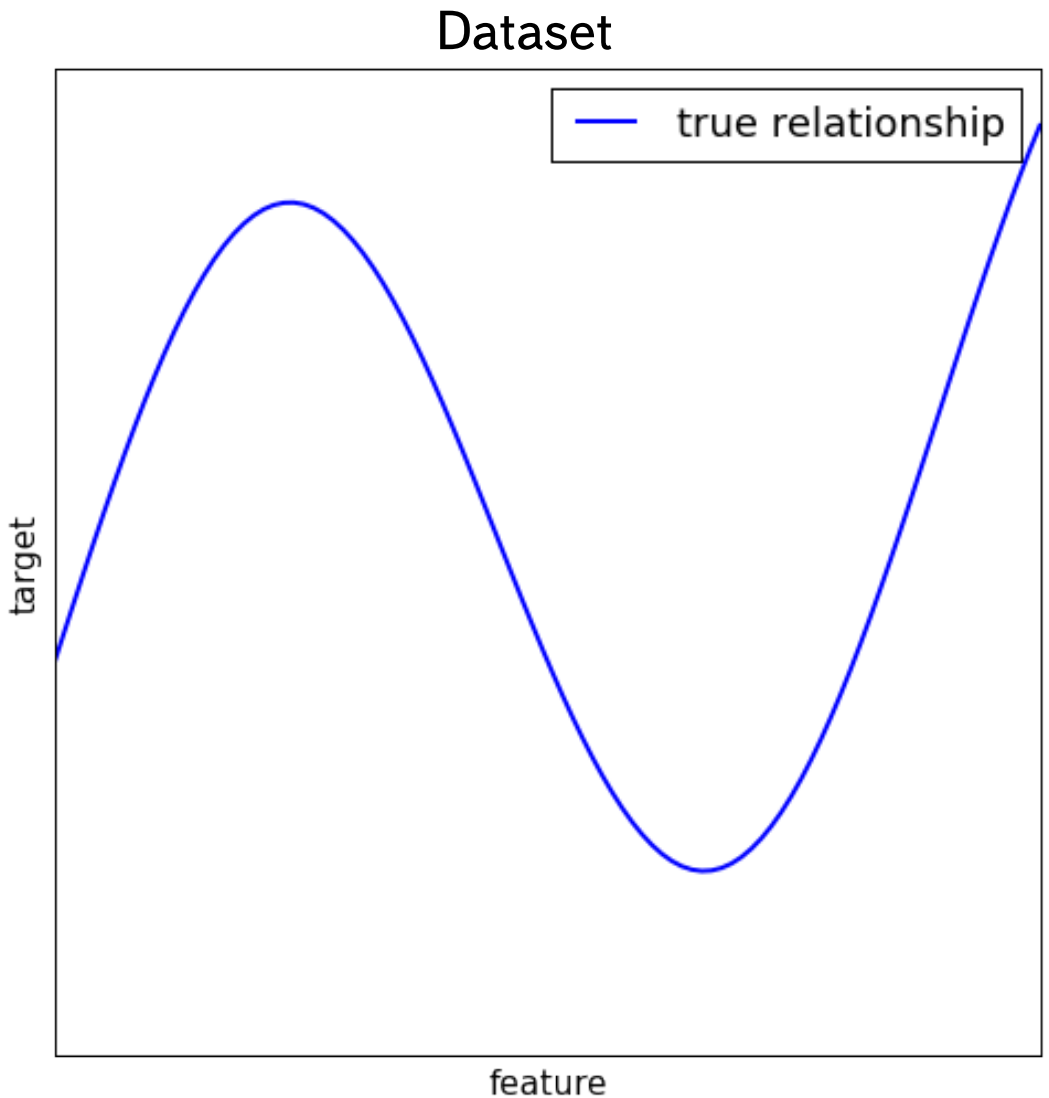
By taking best performing classifier at each point we can achieve $\int \max ROC_1(t), ROC_2(t) dt$.

ROC curve of classifier combination



Interval [B,C]: by selecting classifier1(A) with probability p and classifier2(C) with probability $1-p$ we can obtain AUC as the convex hull of the ROC curves.

Motivation for regression



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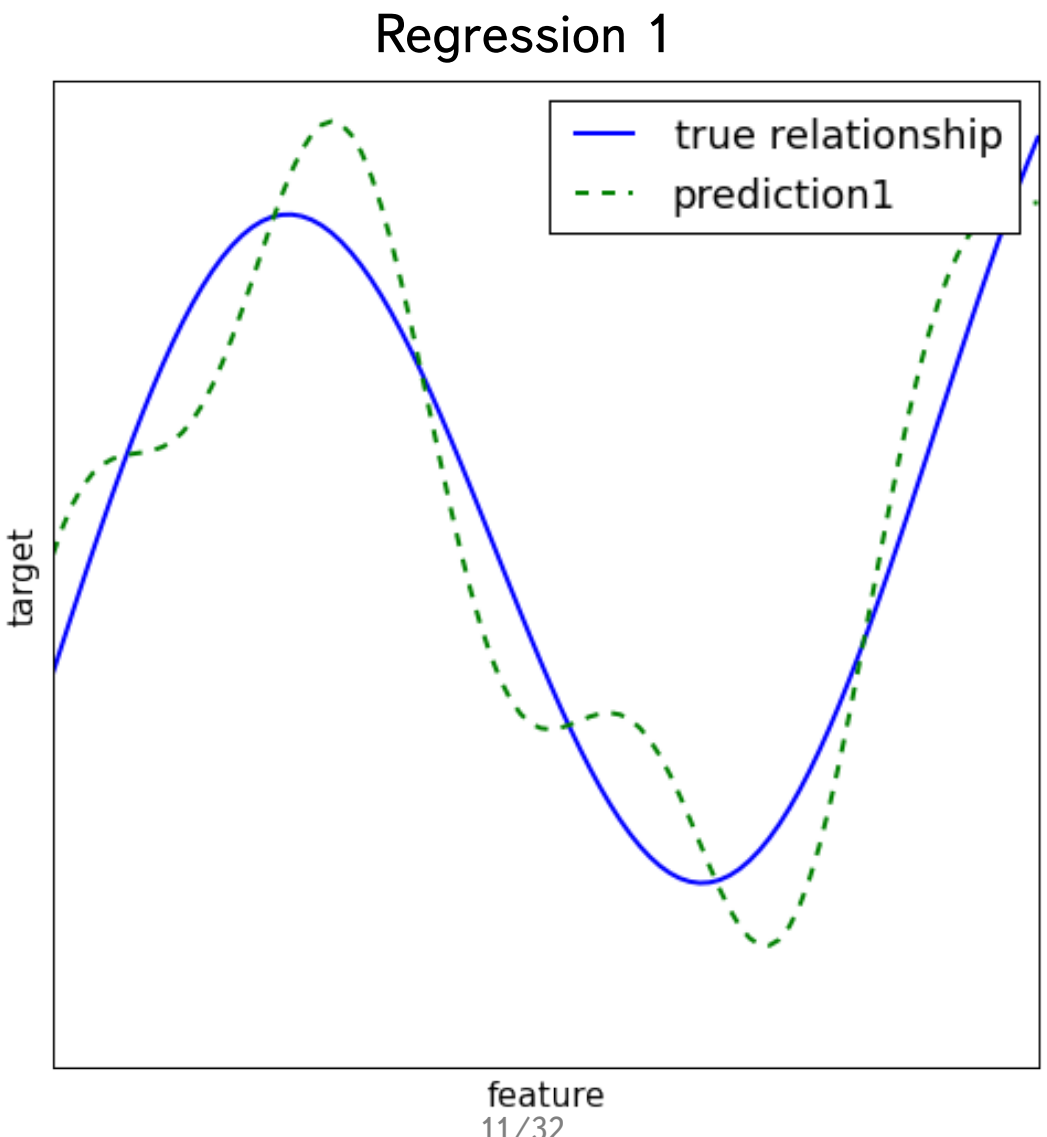

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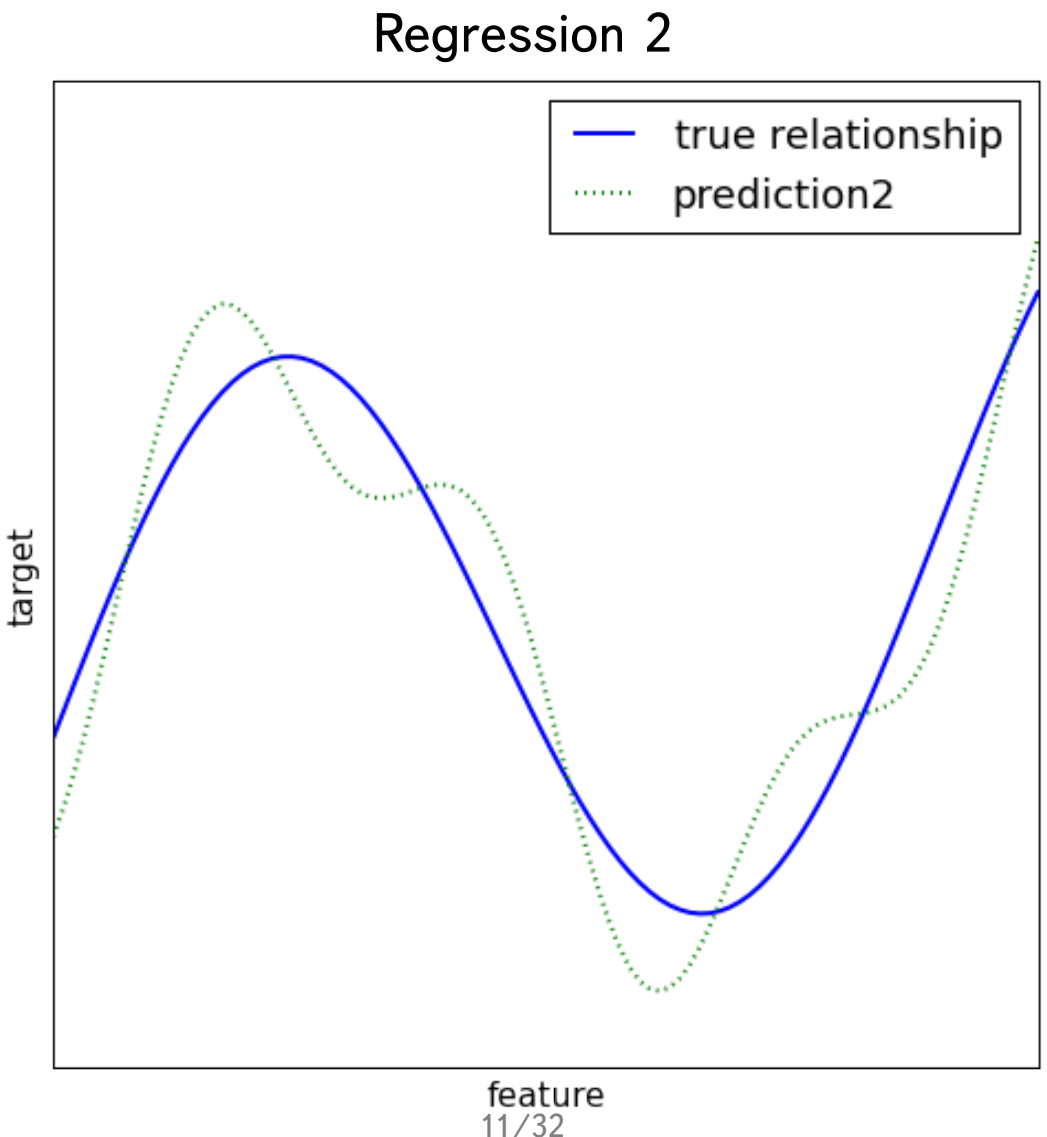
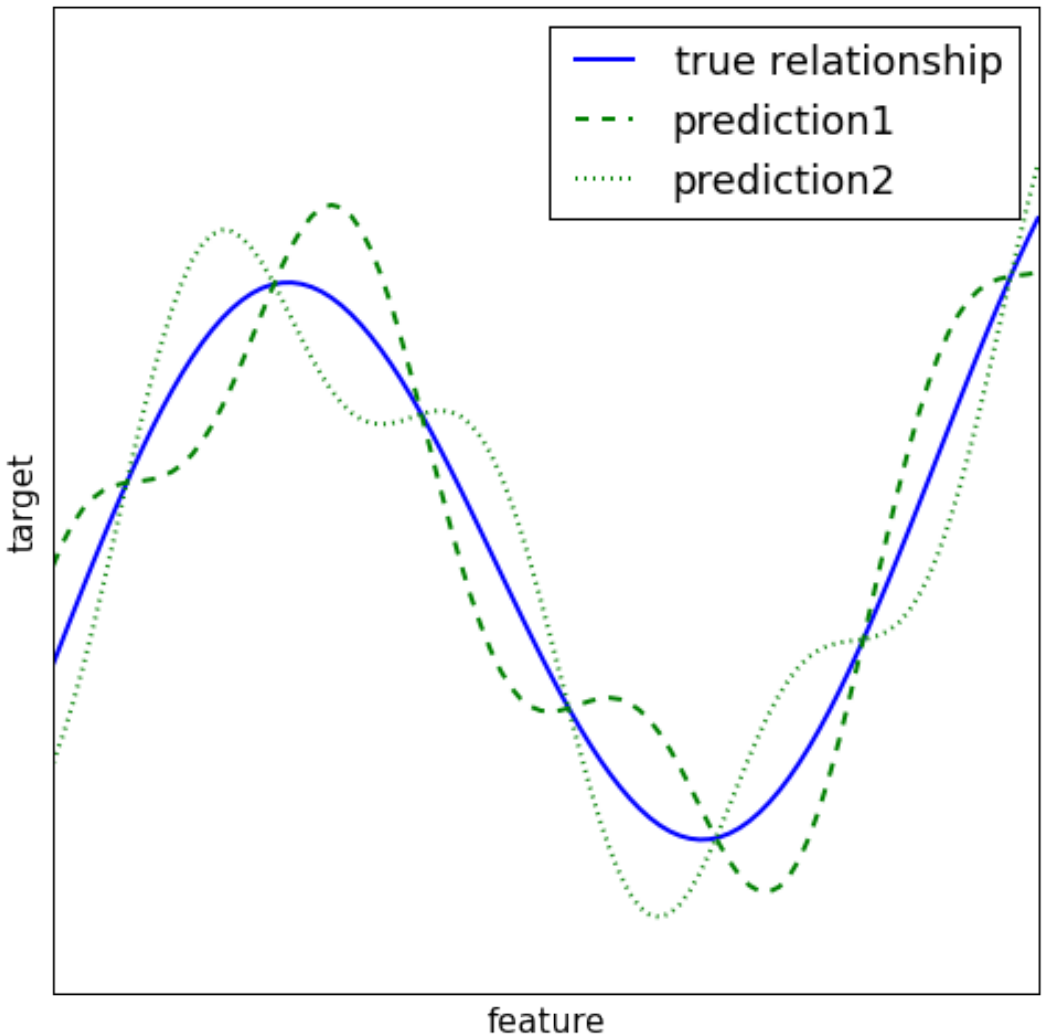


Motivation for regression

Regression 1 and regression 2 combined using averaging



Bias-variance decomposition

Theorem 2 (Bias-variance decomposition)

Unknown relationship $y = f(x) + \varepsilon$ *is reconstructed using a set of points* (x_n, y_n), $n = 1, 2...N$ *as* $\widehat{f}(x)$. *Noise* ε *is independent of any* x, $\mathbb{E}\varepsilon = 0$ *and* $Var[\varepsilon] = \sigma^2$. *Then*

$$\mathbb{E}[\widehat{f} - f]^2 = [\mathbb{E}\widehat{f} - f]^2 + \mathbb{E}[\widehat{f} - \mathbb{E}\widehat{f}]^2$$

$$\mathbb{E}[\widehat{f} - y]^2 = [\mathbb{E}\widehat{f} - f]^2 + \mathbb{E}[\widehat{f} - \mathbb{E}\widehat{f}]^2 + \sigma^2$$

Essentially this means:

$$MSE = \text{bias}^2 + \text{variance} + \text{irreducible error}$$

Different models of ensemble have different bias and variance deviations, which we hope to average away.

Comment: $\mathbb{E}$ is mathematical expectation over different training sets.

Proof of bias-variance decomposition (2)

$$\mathbb{E}\left(\widehat{f}-f\right)^2=\mathbb{E}\left(\widehat{f}-\mathbb{E}\widehat{f}+\mathbb{E}\widehat{f}-f\right)^2=\mathbb{E}\left(\widehat{f}-\mathbb{E}\widehat{f}\right)^2+\left(\mathbb{E}\widehat{f}-f\right)^2$$
$$+2\mathbb{E}\left[(\widehat{f}-\mathbb{E}\widehat{f})(\mathbb{E}\widehat{f}-f)\right]$$
$$=\mathbb{E}\left(\widehat{f}-\mathbb{E}\widehat{f}\right)^2+\left(\mathbb{E}\widehat{f}-f\right)^2$$

We used that $(\mathbb{E}\widehat{f}-f)$ is a constant number and hence $\mathbb{E}\left[(\widehat{f}-\mathbb{E}\widehat{f})(\mathbb{E}\widehat{f}-f)\right]=(\mathbb{E}\widehat{f}-f)\mathbb{E}(\widehat{f}-\mathbb{E}\widehat{f})=0$.

$$\begin{aligned}\mathbb{E}\left(\widehat{f}-y\right)^2 &= \mathbb{E}\left(\widehat{f}-f-\varepsilon\right)^2=\mathbb{E}\left(\widehat{f}-f\right)^2+\mathbb{E}\varepsilon^2-2\mathbb{E}\left[(\widehat{f}-f)\varepsilon\right]\\ &= \mathbb{E}\left(\widehat{f}-\mathbb{E}\widehat{f}\right)^2+\left(\mathbb{E}\widehat{f}-f\right)^2+\sigma^2\end{aligned}$$

We used that $\mathbb{E}\left[(\widehat{f}-f)\varepsilon\right]=\mathbb{E}\left[(\widehat{f}-f)\right]\mathbb{E}\varepsilon=0$ since ε is independent of x.

Diversity

What is a good ensemble?

A good ensemble is the one that consists of accurate predictors that make errors in different regions of input space.

Definition 3

Diversity is a property that characterizes complementarity of base learner errors. It is greater when, all other factors being equal, the classifiers that make incorrect decisions for a given example spread their decisions more evenly over the possible incorrect decisions.

- A lot of diversity definitions exist (see [Zhou, 2012])
- No universal diversity definition yet found.

Ambiguity decomposition

Theorem 4 (Ambiguity decomposition)

Let $F(x) = \sum_{k=1}^{K} \alpha_k f_k(x)$, *where* $\sum_{k=1}^{K} \alpha_k = 1$ *and* $\alpha_k \geq 0$, $k = 1, 2, ...K$. *Then for every instance:*

$$(F - y)^2 = \sum_{k=1}^{K} [\alpha_k (f_k - y)] - \sum_{k=1}^{K} [\alpha_k (f_k - F)^2]$$

Implications:

- ensemble loss is less or equal than weighted loss of individual learners.
- the factor that increases accuracy is ambiguity of individual forecasts.

Shortcoming of this metric: when accuracy increases, ambiguity also decreases and vice versa.

Proof of ambiguity decomposition (4)

$$\begin{aligned}\sum_{k=1}^{K}\alpha_k(f_k-y)^2 &= \sum_{k=1}^{K}\alpha_k(f_k-F+F-y)^2\\ &= \sum_{k=1}^{K}\alpha_k\left[(f_k-F)^2+(F-y)^2+2(f_k-F)(F-y)\right]\\ &= \sum_{k=1}^{K}\alpha_k(f_k-F)^2+(F-y)^2\end{aligned}$$

since, by definition $F=\sum_{k=1}^{K}\alpha_k f_k$. So it follows that

$$(F-y)^2=\sum_{k=1}^{K}\alpha_k(f_k-y)^2-\sum_{k=1}^{K}\alpha_k(f_k-F)^2$$

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Bagging

- Random selection of
  - samples (with replacement)
  - features (without replacement)
- During bootstrap approximately $1 - 1/e \approx 2/3$ samples are retained and $1/e \approx 1/3$ samples left out for large training sets.

Random forests

Input: training dataset $TDS = \{(x_i, y_i),\ 1 = 1, 2, ...n\}$; the number of trees B and the size of feature subsets m.

1. for $b = 1, 2, ...B$:
   1. generate random training dataset TDS^b of size n by sampling (x_i, y_i) pairs from TDS with replacement.
   2. build a tree using TDS^b training dataset with feature selection for each node from random subset of features of size m (generated individually for each node).
2. Evaluate the quality by assigning output to x_i, $i = 1, 2, ...n$ using majority vote (classification) or averaging (regression) among trees with $b \in \{b : (x_i, y_i) \notin T^b\}$

Output: B trees. Classification is done using majority vote and regression using averaging of B outputs.

Comments

- Random forests use random selection on both samples and features
- Left out samples are used for evaluation of model performance.
- Less interpretable than individual trees
- Pro: Parallel implementation
- Contra: different trees are not targeted to correct mistakes of each other

Forward stagewise additive modeling

Input: training dataset (x_i, y_i), $i = 1, 2, ...n$; loss function $L(f, y)$, general form of additive classifier $h(x, \gamma)$ (dependent from parameter γ) and the number M of successive additive approximations.

1. Fit initial approximation $f^0(x)$ (might be taken $f^0(x) \equiv 0$)
2. For $m = 1, 2, ...M$:
    1. find next best classifier
$$(c_m, \gamma_m) = \arg\min \sum_{i=1}^{n} L(f_{m-1}(x_i) + c_m h(x, \gamma_m),\ y_i)$$
    2. set
$$f_m(x) = f_{m-1}(x) + c_m h(x, \gamma_m)$$

Output: approximation function $f^M(x) = f^0(x) + \sum_{j=1}^{M} c_j h(x, \gamma_m)$

Adaboost algorithm is obtained for $L(y, f(x)) = e^{-yf(x)}$

Adaboost (discrete version)

Assumptions: loss function $L(y, f(x)) = e^{-yf(x)}$
Input: training dataset (x_i, y_i), $i = 1, 2, ...n$; number of additive weak classifiers M, a family of weak classifiers $h(x)$, outputting only +1 or -1 (binary classification) and trainable on weighted datasets.

1. Initialize observation weights $w_i = 1/n$, $i = 1, 2, ...n$.
2. for $m = 1, 2, ...M$:
    1. fit $h^m(x)$ to training data using weights w_i
    2. compute weighted misclassification rate:

$$E_m = \frac{\sum_{i=1}^n w_i \mathbb{I}[h^m(x) \neq y_i]}{\sum_{i=1}^n w_i}$$

    3. compute $\alpha_m = \ln((1 - E_m)/E_m)$
    4. increase all weights, where misclassification with $h^m(x)$ was made:

$$w_i \leftarrow w_i e^{\alpha_m},\ i \in \{i : h^m(x_i) \neq y_i\}$$

Output: composite classifier $f(x) = \text{sign}\left(\sum_{m=1}^M \alpha_m h^m(x)\right)$

Adaboost derivation

Set initial approximation $f^0(x) \equiv 0$.
Apply forward stagewise algorithm for $m = 1, 2, ...M$:

$$\begin{aligned}(c_m, h^m) &= \arg\min_{c_m, h^m} \sum_{i=1}^{n} L(f_{m-1}(x_i) + c_m h^m(x), y_i) \\ &= \arg\min_{c_m, h^m} \sum_{i=1}^{n} e^{-y_i f_{m-1}(x_i)} e^{-c_m y_i h^m(x)} \\ &= \arg\min_{c_m, h^m} \sum_{i=1}^{n} w_i^m e^{-c_m y_i h^m(x_i)}, \quad w_i^m = e^{-y_i f_{m-1}(x_i)}\end{aligned}$$

Since $c_m \geq 0$ and $y_i h^m(x_i) \in \{-1, +1\}$ minimum with respect to $h^m(x)$ is attained at

$$h^m(x_i) = \arg\min_h \sum_{i=1}^{n} w_i^m \mathbb{I}[h(x_i) \neq y_i]$$

Adaboost derivation

Denote $F(c_m) = \sum_{i=1}^n w_i^m \exp(-c_m y_i h^m(x_i))$. Then

$$\frac{\partial F(c_m)}{\partial c_m} = -\sum_{i=1}^n w_i^m e^{-c_m y_i h^m(x_i)} y_i h^m(x_i) = 0$$

$$-\sum_{i:h^m(x_i)=y_i} w_i^m e^{-c_m} + \sum_{i:h^m(x_i)\neq y_i} w_i^m e^{c_m} = 0$$

$$e^{2c_m} = \frac{\sum_{i:h^m(x_i)=y_i} w_i^m}{\sum_{i:h^m(x_i)\neq y_i} w_i^m}$$

$$c_m = \frac{1}{2}\ln\frac{\left(\sum_{i:h^m(x_i)=y_i} w_i^m\right)/\left(\sum_{i=1}^n w_i^m\right)}{\left(\sum_{i:h^m(x_i)\neq y_i} w_i^m\right)/\left(\sum_{i=1}^n w_i^m\right)} = \frac{1}{2}\ln\frac{1-E_m}{E_m} = \frac{1}{2}\alpha_m,$$

$$E_m = \frac{\sum_{i=1}^n w_i^m \mathbb{I}[h^m(x_i)\neq y_i]}{\sum_{i=1}^n w_i^m}$$

Adaboost derivation

Weights recalculation:

$$w_i^{m+1} \stackrel{df}{=} e^{-y_i f_m(x_i)} = e^{-y_i f_{m-1}(x_i)} e^{-y_i c_m h^m(x_i)}$$

Noting that $-y_i h^m(x_i) = 2\mathbb{I}[h^m(x_i) \neq y_i] - 1$, we can rewrite:

$$\begin{aligned} w_i^{m+1} &= e^{-y_i f_{m-1}(x_i)} e^{c_m(2\mathbb{I}[h^m(x_i)\neq y_i]-1)} = \\ &= w_i^m e^{2c_m\mathbb{I}[h^m(x_i)\neq y_i]} e^{-c_m} \propto w_i^m e^{2c_m\mathbb{I}[h^m(x_i)\neq y_i]} \end{aligned}$$

On the last step we used the property that classification result is not affected by multiplication of all weights by constant.

Gradient boosting

- For general loss function L forward stagewise algorithm can be solved explicitly in rare cases. In general gradient boosting is applied.
- Gradient boosting is analogous to steepest descent:
  - function approximation is composed of sums of approximations, each of which approximates $\partial L/\partial f$.

Gradient boosting

Input: training dataset (x_i, y_i), $i = 1, 2, ...n$; loss function $L(f, y)$ and the number M of successive additive approximations.

1. Fit initial approximation $f^0(x)$ (might be taken $f^0(x) \equiv 0$)
2. For each step $m = 1, 2, ...M$:
   1. calculate derivatives $z_i = -\frac{\partial L(r,y)}{\partial r}|_{r=f^{m-1}(x)}$
   2. train additive approximation with classifier h^m on (x_i, z_i), $i = 1, 2, ...n$ with some loss function $\sum_{i=1}^{n} \mathcal{L}\left(h^m(x_i), z_i\right)$
   3. solve univariate optimization problem:

$$\sum_{i=1}^{n} L\left(f^{m-1}(x_i) + c_m h^m(x_i), y_i\right) \to \min_{c_m \in \mathbb{R}_+}$$

   4. set $f^m(x) = f^{m-1}(x) + c_m h^m(x)$

Output: approximation function $f^M(x) = f^0(x) + \sum_{m=1}^{M} c_m h^m(x)$

Gradient boosting of trees

Input: training dataset (x_i, y_i), $i = 1, 2, ...n$; loss function $L(f, y)$ and the number M of successive additive approximations.

1. Fit constant initial approximation $f^0(x)$: $f^0(x) = \arg\min_\gamma \sum_{i=1}^n L(\gamma, y_i)$
2. For each step $m = 1, 2, ...M$:
   1. calculate derivatives $z_i = -\frac{\partial L(r,y)}{\partial r}|_{r=f^{m-1}(x)}$
   2. train regression tree h^m on (x_i, z_i), $i = 1, 2, ...n$ with some loss function $\sum_{i=1}^n \mathcal{L}(h^m(x_i), z_i)$ and extract terminal regions R_{jm}, $j = 1, 2, ...J_m$.
   3. for each terminal region R_{jm}, $j = 1, 2, ...J_m$ solve univariate optimization problem:

$$\gamma_{jm} = \arg\min_\gamma \sum_{x_i \in R_{jm}} L(f^{m-1}(x_i) + \gamma, y_i)$$

   4. update $f^m(x) = f^{m-1}(x) + \sum_{j=1}^{J_m} \gamma_{jm} \mathbb{I}[x \in R_{jm}]$

Output: approximation function $f^M(x)$

Modification of boosting for trees

- Compared to first method of gradient boosting, boosting of regression trees finds additive coefficients individually for each terminal region R_{jm}, not globally for the whole classifier $h^m(x)$.
- This is done to increase accuracy: forward stagewise algorithm cannot be applied to find R_{jm}, but it can be applied to find γ_{jm}, because second task is solvable for arbitrary L.

Loss function selection

- Usually $\mathcal{L}(h,z) = (h-z)^2$, though using absolute loss or Huber function loss makes procedure more robust to outliers.
- $L(\widehat{y},y)$ specification:
  - in regression $L(\widehat{y},y)$ is set to regression loss function:
    - squared deviation, absolute deviation, Huber loss
    - when $L(\widehat{y},y) = (\widehat{y}-y)^2$ method is called *L2Boost*.
  - in classification $L(f,y)$ is set to margin loss function:
    - exponential $L(f,y) = e^{-fy}$ or log-loss $L(f,y) = \ln(1+e^{-fy})$.
    - log-loss optimization with approximate solution from single step of Newton-Rhapson method is called *LogitBoost*
    - log-loss optimization yields not only classes, but also class probabilities.