Introduction to Machine Learning and Data Mining
Ensemble classifiers

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Outline

Outline

Bias-variance decomposition

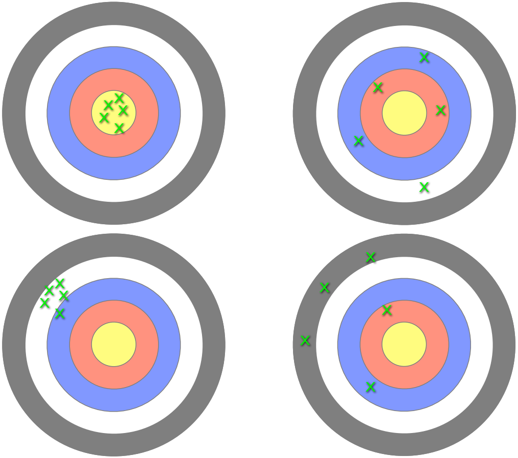


Рис. 1: *Source: Machine Learning – The Art and Science of Algorithms that Make Sense of Data*

Bias-variance decomposition

- Regression case ($x_1, \ldots, x_n$ and $y_i \in \mathbb{R}$)

$$\mathbf{E}[(y - \hat{f}(x))^2] = (\mathbf{Bias}[\hat{f}(x)])^2 + \mathbf{Var}[\hat{f}(x)] + \sigma^2, \text{ under condition}$$

$y = f(x) + \varepsilon$, where $\mathbf{E}(\varepsilon) = 0$ and $\mathbf{Var}(\varepsilon) = \sigma^2$ (not necessary normal distribution)

$$\mathbf{Bias}[\hat{f}(x)] = \mathbf{E}[\hat{f}(x) - f(x)]$$

$$\mathbf{Var}[\hat{f}(x)] = \mathbf{E}[\hat{f}(x)^2] - (\mathbf{E}[\hat{f}(x)])^2$$

Outline

Bagging (BootstrapAggregation)

(Breiman, 1996), ссылка

Let us consider a training set $\mathcal{L} = \{(\mathbf{x}_i, y_i), 1, \dots n\},$ где
$y_i \in \mathbb{R}$ (regression problem) or $y_i \in \{1, \dots k\}$ (classification problem).

Let us generate B training sets $\mathcal{L}^b$ of length n with replacements $\mathcal{L}$.

$$\mathcal{L}^b = \{(\mathbf{x}_i^b, y_i^b), i = 1, 2, \dots, n\}, \text{ где}$$

$b = 1, 2, \dots, B$, and $p_i = 1/n$ is the probability of each pair (x_i, y_i) to be chosen from $\mathcal{L}$.

37 % $\left(1-\frac{1}{n}\right)^n \quad n \to \infty \quad = e^{-1}$ 1/e

Bagging over classification trees

Let us build a tree $\mathcal{T}^b$ for each set $\mathcal{L}^b$.
If $(\mathbf{x}, y) \in \mathcal{L} \setminus \mathcal{L}^b$, then the pair $(\mathbf{x}, y)$ is out-of-bag.
37% of examples for each $\mathcal{L}^b$ do not contribute to the tree training process
For $\mathbf{x}_i \notin \mathcal{L}^b$ we predict its class by applying the tree $\mathcal{T}^b$: $\mathcal{T}^b(\mathbf{x})$.
Let us assume that for $n_i \leq B$ trees, the example $\mathbf{x}_i$ is out-of-bag, then its class distribution vector is as follows:

$$\hat{p}(x_i) = (\hat{p_1}(x_i), \hat{p_2}(x_i), \ldots, \hat{p_K}(x_i))^T$$

OOB-classifier

$$C_{bag}(x_i) = \arg\max_k \hat{p}_k(x_i)$$

Error-rate:

$$PE = \frac{1}{n}\sum_{i=1}^{n}[C_{bag}(\mathbf{x}_i) \neq y_i]$$

Example

Spambase: 57 features for 4601 messages, two classes: spam (1813 messages) or e-mail (2788 messages). Imbalance ratio $1813/4601 = 0{,}394$.

Decision tress: stumps, trees with 4 nodes, 8 nodes and fully-grown trees. Bagging for B form 10 to 200 with the step size 25.

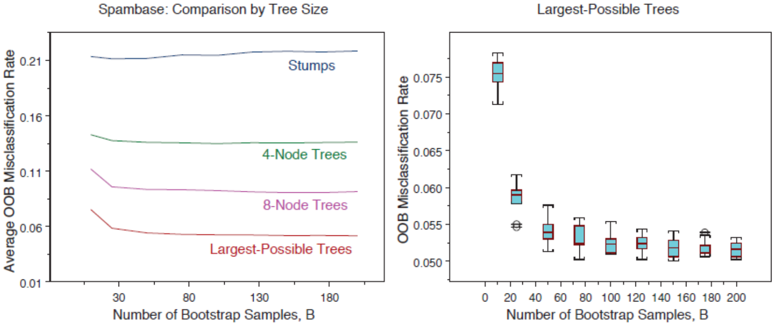


Рис. 2: *Source: Modern Multivariate Statistical Techniques*

Bagging over decision trees

Let us build a decision tree $\mathcal{T}^b$ for each bagging sample $\mathcal{L}^b$.
For $\mathbf{x}$ we obtain the prediction by the tree $\mathcal{T}^b$ as follows: $\hat{\mu}^b(\mathbf{x})$.

OOB-estimate

$$\hat{\mu}_{bag}(\mathbf{x}) = \frac{1}{B}\sum_{b=1}^{B}\hat{\mu^b}(x)$$

Errors rate:

$$PE_{bag} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{\mu}_{bag}(\mathbf{x}_i))^2$$

Outline

Boosting

[Schapire (1990) link], Freund (1995) link]

Weak (or base) classifier correctly classifies examples as $\{+1, -1\}$ more than in 50% cases.
Boosting of the algorithms combines M base classifiers $C_1, C_2, \ldots, C_M$.
For an object $\mathbf{x}$, "boosted" classifier is as follows:

$$C_\alpha(\mathbf{x}) = sign\{f_\alpha(\mathbf{x})\}, \text{где}$$

$f_\alpha(\mathbf{x}) = \sum\limits_{j=1}^{M} \left(\frac{\alpha_j}{\sum_k \alpha_k}\right) C_j(\mathbf{x})$, $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_M)$ is the coefвектор коэффициентов.

Example

$M = 4$

$$C_1(\text{e-mail}) = \begin{cases} +1 & \text{if the message contains the word “money”} \\ -1 & \text{otherwise} \end{cases}$$

$$C_2(\text{e-mail}) = \begin{cases} +1 & \text{if the message contains the word “free”} \\ -1 & \text{otherwise} \end{cases}$$

$$C_3(\text{e-mail}) = \begin{cases} +1 & \text{if the message contains the word “order”} \\ -1 & \text{otherwise} \end{cases}$$

$$C_4(\text{e-mail}) = \begin{cases} +1 \text{ if the message contains the word “credit”} \\ -1 \text{ otherwise} \end{cases}$$

$$f(\text{e-mail}) = 0,2C_1(\text{e-mail}) + 0,1C_2(\text{e-mail}) + 0,4C_3(\text{e-mail}) + 0,3C_4(\text{e-mail})$$

The message contains words “money”, “order”, and “credit”

$$f(\text{e-mail}) = 0,2 - 0,1 + 0,4 + 0,3 = 0,8$$

$sign\{f(\text{e-mail})\} = sign\{0,8\} = +1 \Rightarrow \text{spam}$

AdaBoost

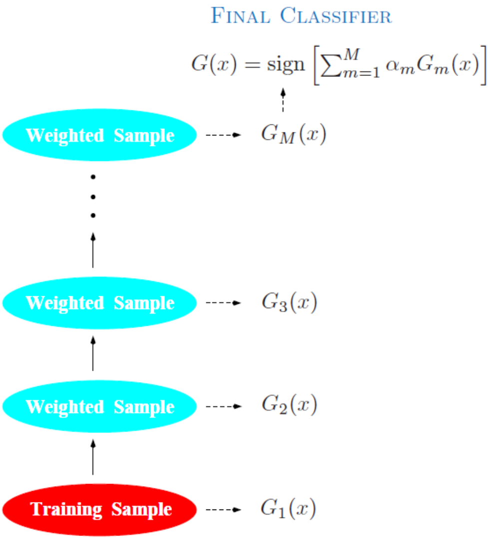


Рис. 3: *Source: Modern Multivariate Statistical Techniques*

AdaBoost.M1

1. Input: $\mathcal{L} = \{(\mathbf{X}_i, Y_i), i = 1, 2, \ldots, n\}$, $Y_i \in \{-1, +1\}$, $i = 1, 2, \ldots, n$, $\mathcal{C} = \{C_1, C_2, \ldots, C_M\}$, T = number of iterations.
2. Initialize the weight vector: Set $\mathbf{w}_1 = (w_{11}, \cdots, w_{n1})^\tau$, where $w_{i1} = 1/n$, $i = 1, 2, \ldots, n$.
3. For $t = 1, 2, \ldots, T$:
   - Select a weak classifier $C_{j_t}(\mathbf{x}) \in \{-1, +1\}$ from $\mathcal{C}$, $j_t \in \{1, 2, \ldots, M\}$, and train it on the learning set $\mathcal{L}$, where the ith observation $(\mathbf{X}_i, Y_i)$ has (normalized) weight w_{it}, $i = 1, 2, \ldots, n$.
   - Compute the weighted prediction error:
   $$PE_t = PE(\mathbf{w}_t) = \mathrm{E}_w\{I_{[Y_i \neq C_{j_t}(\mathbf{X}_i)]}\} = \left(\frac{\mathbf{w}_t^\tau}{\mathbf{1}_n^\tau \mathbf{w}_t}\right)\mathbf{e}_t,$$
   where E_w indicates taking expectation with respect to the probability distribution of $\mathbf{w}_t = (w_{1t}, \cdots, w_{nt})^\tau$, and $\mathbf{e}_t$ is an n-vector with ith entry $[\mathbf{e}_t]_i = I_{[Y_i \neq C_{j_t}(\mathbf{X}_i)]}$.
   - Set $\beta_t = \frac{1}{2}\log\left(\frac{1-PE_t}{PE_t}\right)$.
   - Update weights:
   $$w_{i,t+1} = \frac{w_{it}}{W_t}\exp\{2\beta_t I_{[Y_i \neq C_{j_t}(\mathbf{X}_i)]}\}, \quad i = 1, 2, \ldots, n,$$
   where W_t is a normalizing constant needed to ensure that the vector $\mathbf{w}_{t+1} = (w_{1,t+1}, \cdots, w_{n,t+1})^\tau$ represents a true weight distribution over $\mathcal{L}$; that is, $\mathbf{1}_n^\tau \mathbf{w}_{t+1} = 1$.
4. Output: $\mathrm{sign}\{f(\mathbf{x})\}$, where $f(\mathbf{x}) = \sum_{t=1}^T \beta_t C_{j_t}(\mathbf{x}) = \sum_{j=1}^M \alpha_j C_j(\mathbf{x})$, and $\alpha_j = \sum_{t=1}^T \beta_t I_{[j_t = j]}$.

Рис. 4: *Source: Modern Multivariate Statistical Techniques*

AdaBoost.M1

1. Initialize the observation weights $w_i = 1/N,\ i = 1, 2, \ldots, N$.
2. For $m = 1$ to M:
   (a) Fit a classifier $G_m(x)$ to the training data using weights w_i.
   (b) Compute
   $$\mathrm{err}_m = \frac{\sum_{i=1}^{N} w_i I(y_i \neq G_m(x_i))}{\sum_{i=1}^{N} w_i}.$$
   (c) Compute $\alpha_m = \log((1 - \mathrm{err}_m)/\mathrm{err}_m)$.
   (d) Set $w_i \leftarrow w_i \cdot \exp[\alpha_m \cdot I(y_i \neq G_m(x_i))],\ i = 1, 2, \ldots, N$.
3. Output $G(x) = \mathrm{sign}\left[\sum_{m=1}^{M} \alpha_m G_m(x)\right]$.

Рис. 5: *Source: Elements of Statistical Learning*

AdaBoost: Example

Данные: Solubility data 5631×71, 2 classes (soluble and insoluble compounds)

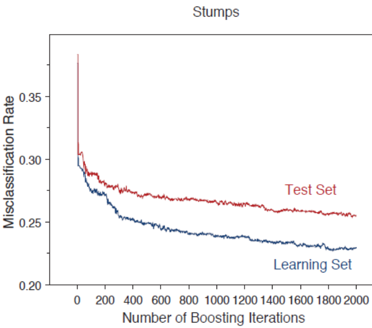


Рис. 6: *Source: Modern Multivariate Statistical Techniques*

Boosting for regression

1. Set $\hat{f}(x) = 0$ and $r_i = y_i$ for all i in the training set.
2. For $b = 1, 2, \ldots, B$, repeat:
   (a) Fit a tree $\hat{f}^b$ with d splits ($d + 1$ terminal nodes) to the training data (X, r).
   (b) Update $\hat{f}$ by adding in a shrunken version of the new tree:
   $$\hat{f}(x) \leftarrow \hat{f}(x) + \lambda \hat{f}^b(x). \tag{0}$$
   (c) Update the residuals,
   $$r_i \leftarrow r_i - \lambda \hat{f}^b(x_i). \tag{1}$$
3. Output the boosted model,
$$\hat{f}(x) = \sum_{b=1}^{B} \lambda \hat{f}^b(x). \tag{2}$$

Рис. 7: *Source: Introduction to Statistical Learning*

Gradient boosting

Greedy Function Approximation: A Gradient Boosting Machine, Friedman (1999-2001)

Idea:

use the loss gradient by the added function during the training phase

Implementation with the regularisation: XGBoost library

Outline

Random Forest

Breiman (2001), статья

Idea:

The average of B i.i.d. random variables, each with variance σ^2, has variance $\frac{1}{B}\sigma^2$. If the variables are i.d. (but not necessarily independent) with positive pair-wise correlation ρ, the variance of their mean:

$$\rho\sigma^2 + \frac{(1-\rho)}{B}\sigma^2.$$

What is happening when B grows?

Random Forest

Breiman (2001), статья

1. For $b = 1$ to B:

   (a) Draw a bootstrap sample $\mathbf{Z}^*$ of size N from the training data.

   (b) Grow a random-forest tree T_b to the bootstrapped data, by recursively repeating the following steps for each terminal node of the tree, until the minimum node size n_{min} is reached.

      i. Select m variables at random from the p variables.

      ii. Pick the best variable/split-point among the m.

      iii. Split the node into two daughter nodes.

2. Output the ensemble of trees $\{T_b\}_1^B$.

To make a prediction at a new point x:

Regression: $\hat{f}_{\rm rf}^B(x) = \frac{1}{B}\sum_{b=1}^B T_b(x)$.

Classification: Let $\hat{C}_b(x)$ be the class prediction of the bth random-forest tree. Then $\hat{C}_{\rm rf}^B(x) = \textit{majority vote}\ \{\hat{C}_b(x)\}_1^B$.

Рис. 8: *Source: Elements of Statistical Learning*

Comparison of boosting, bagging, and random forest

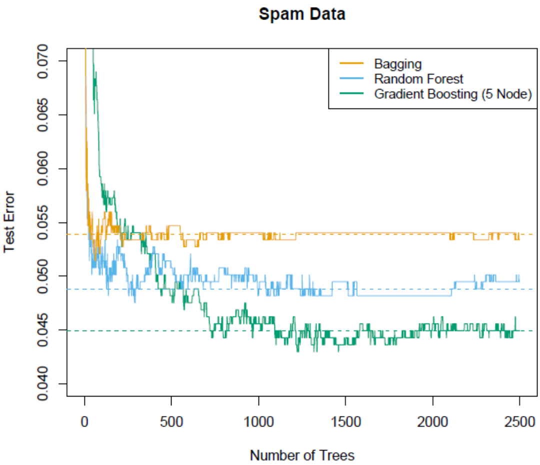


FIGURE 15.1. *Bagging, random forest, and gradient boosting, applied to the spam data. For boosting, 5-node trees were used, and the number of trees were chosen by 10-fold cross-validation (2500 trees). Each "step" in the figure corresponds to a change in a single misclassification (in a test set of 1536).*

Outline

Classic variant

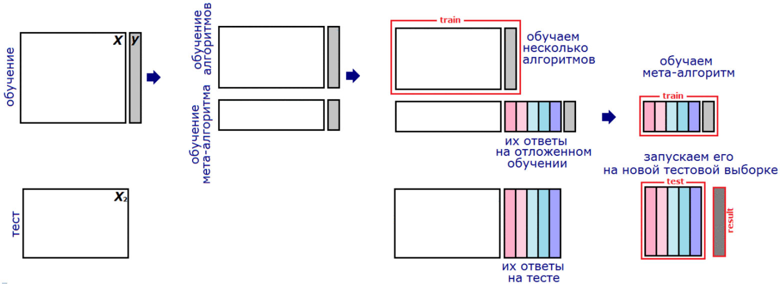


Рис. 10: *Source: Blog of Alexander Diakonov*

Blending
Modification

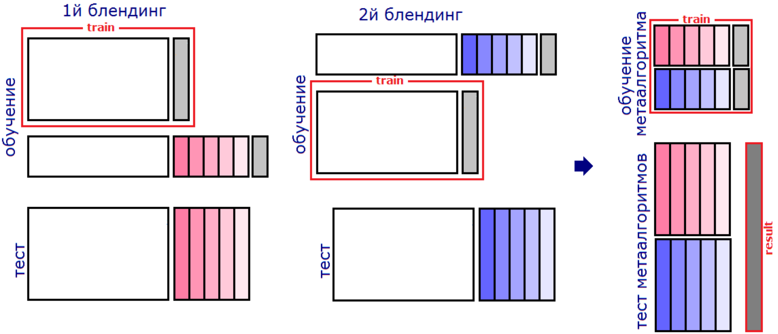


Рис. 11: *Source: Blog Alexander Diakonov*

Stacking or Stacked Generalization

David H. Wolpert: Stacked generalization. Neural Networks 5(2): 241-259 (1992)

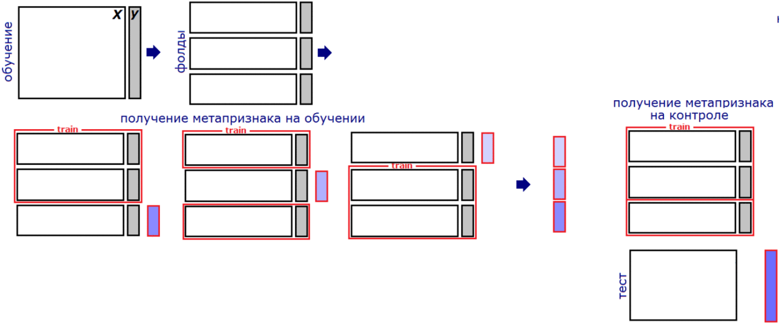


Рис. 12: *Source: Blog Alexander Diakonov*

Stacking or Stacked Generalization

Data source: http://mlbootcamp.ru/

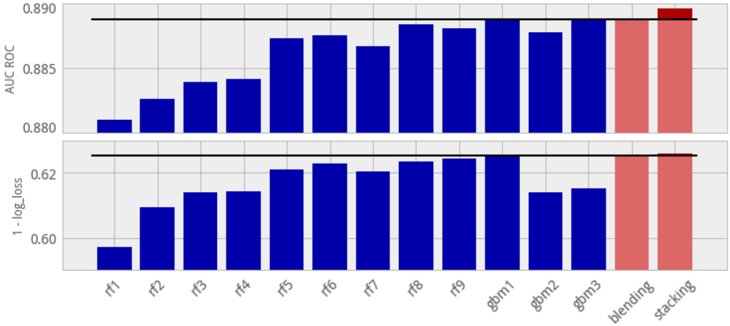


Рис. 13: *Source: Blog Alexander Diakonov*

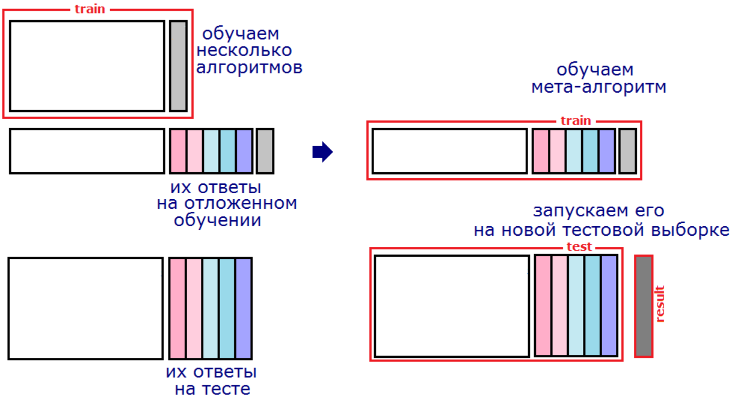


Рис. 14: *Source: Blog Alexander Diakonov*

Stacking or Stacked Generalization

Typical scheme

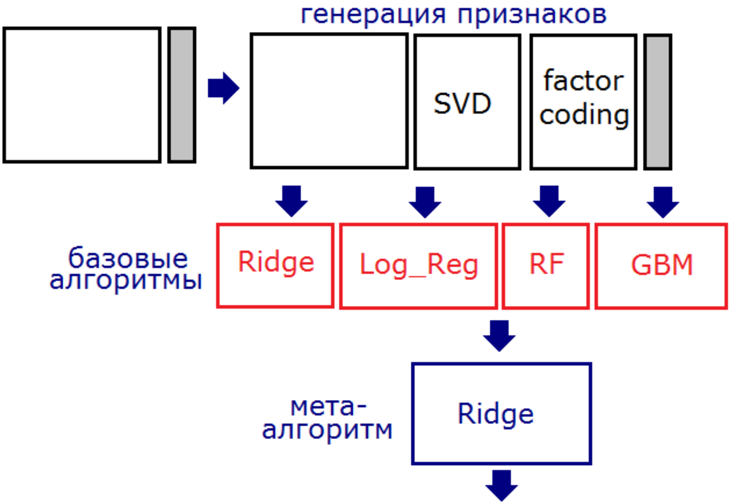


Рис. 15: *Source: Блог Alexander Diakonov*

Yury Kashnitsky, Dmitry I. Ignatov. Can FCA-based Recommender System Suggest a Proper Classifier? ECAI 2014, workshop FCA4AI

Таблица 1: *A sample data set of 10 objects with 4 attributes and 1 binary target class*

G/M	m_1	m_2	m_3	m_4	Label
1	×	×		×	1
2	×			×	1
3		×	×		0
4	×		×	×	1
5	×	×	×		1
6		×	×	×	0
7	×	×	×		1
8			×	×	0
9	×	×	×	×	?
10		×		×	?

Таблица 2: *A classification context*

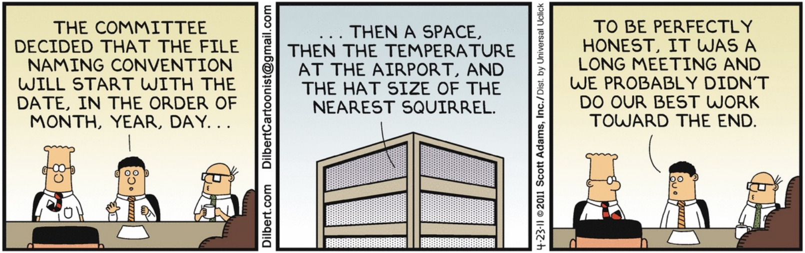
G/C	cl_1	cl_2	cl_3	cl_4
1	×		×	×
2		×	×	
3	×			×
4		×	×	
5	×	×		
6	×	×		×
7		×		×
8		×	×	×

Yury Kashnitsky, Dmitry I. Ignatov. Can FCA-based Recommender System Suggest a Proper Classifier? ECAI 2014, workshop FCA4AI

Таблица 3: *Recommending classifiers for objects from* G_{test}

G_{test}	1^{st} nearest neighbor	2^{nd}	3^{rd}	Neighbors	Classification concept	Recommended classifier
9	4	5	7	$\{4,5,7\}$	$(\{2,4,5,6,7,8\},\{cl_2\})$	cl_2
10	1	6	8	$\{1,6,8\}$	$(\{1,3,6,7,8\},\{cl_4\})$	cl_4

Just for fun или шутки ради



References

- A.J. Izenman, Modern Multivariate Statistical Techniques, Chapter 14

Question and contacts

www.hse.ru/staff/dima

Thank you!

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