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Advanced Machine Learning

Boosting and Stacking

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Slide adapted from
Jing Gao’s SDM 2010 tutorial “On the Power of Ensemble: Supervised and Unsupervised Methods Reconciled”
https://project.dke.maastrichtuniversity.nl/datamining/2013-Slides/lecture-07.ppt

Outline

- Why ensemble learning?
- Supervised learning
  - Methods for Independently Constructing Ensembles
    - Majority Vote, Bagging and Random Forest
  - **Methods for Coordinated Construction of Ensembles**
    - **Boosting, Stacking**

Methods for Coordinated Construction of Ensembles

The key idea is to learn complementary classifiers so that instance classification is realized by taking an weighted sum of the classifiers. This idea is used in two methods:

- Boosting
- Stacking.

Boosting

- Also uses voting/averaging but models are weighted according to their performance
- Iterative procedure: new models are influenced by performance of previously built ones
  - New model is encouraged to become expert for instances classified incorrectly by earlier models
  - Intuitive justification: models should be experts that complement each other

Boosting Example

- Example
  – Record 4 is hard to classify
  – Its weight is increased, therefore it is more likely to be chosen again in subsequent rounds

Original Data	1	2	3	4	5	6	7	8	9	10
Boosting (Round 1)	7	3	2	8	7	9	4	10	6	3
Boosting (Round 2)	5	4	9	4	2	5	1	7	4	2
Boosting (Round 3)	4	4	8	10	4	5	4	6	3	4

AdaBoost.M1

classifier generation

```
Assign equal weight to each training instance.
For each of t iterations:
  Learn a classifier from weighted dataset.
  Compute error e of classifier on weighted dataset.
  If e equal to zero, or e greater or equal to 0.5:
    Terminate classifier generation.
  For each instance in dataset:
    If instance classified correctly by classifier:
       Multiply weight of instance by e / (1 - e).
  Normalize weight of all instances.
```

classification

```
Assign weight of zero to all classes.
For each of the t classifiers:
  Add -log(e / (1 - e)) to weight of class predicted
  by the classifier.
Return class with highest weight.
```

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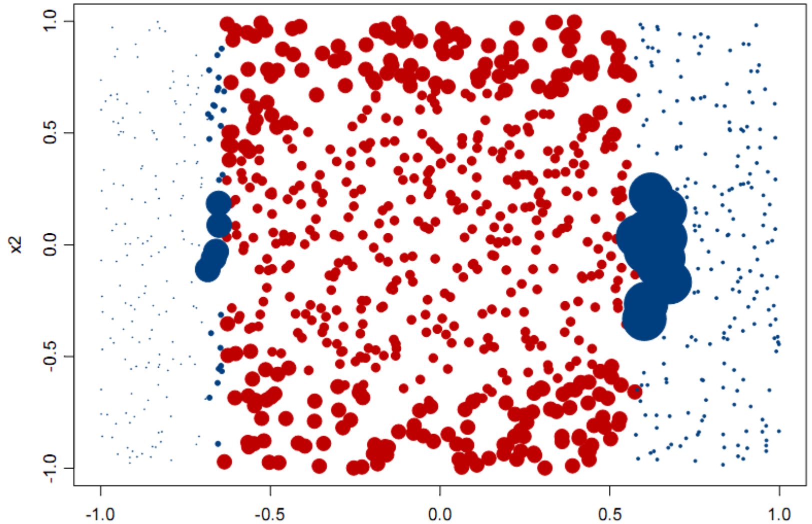
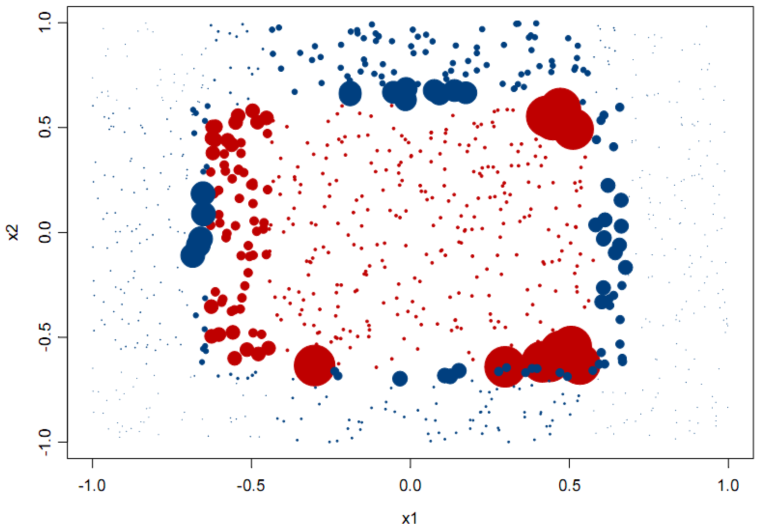
Remarks on Boosting

- Boosting can be applied without weights using re-sampling with probability determined by weights;
- Boosting decreases exponentially the training error in the number of iterations;
- Boosting works well if base classifiers are not too complex and their error doesn't become too large too quickly!
- Boosting reduces the bias component of the error of simple classifiers!

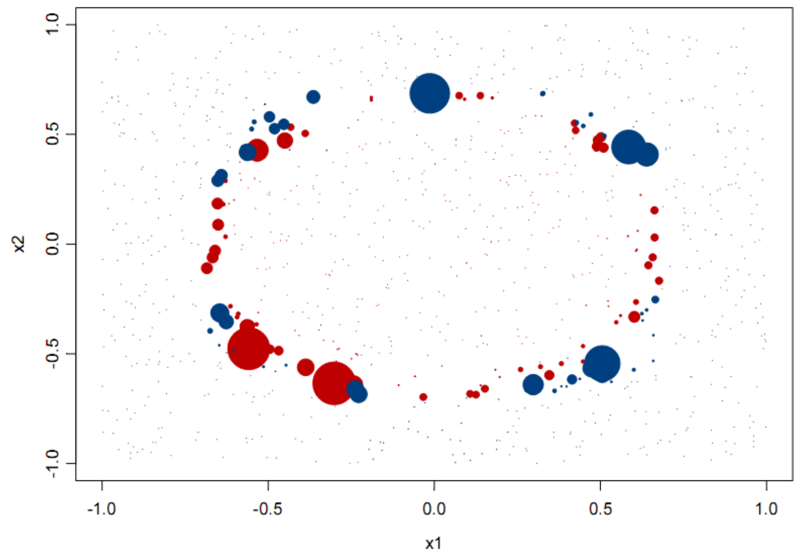


Classifications (colors) and Weights (size) after *1 iteration* Of AdaBoost

3 iterations

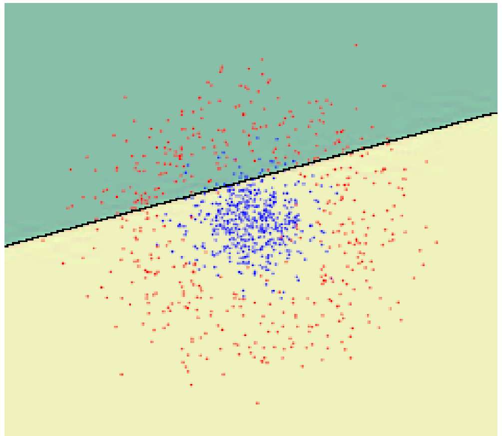


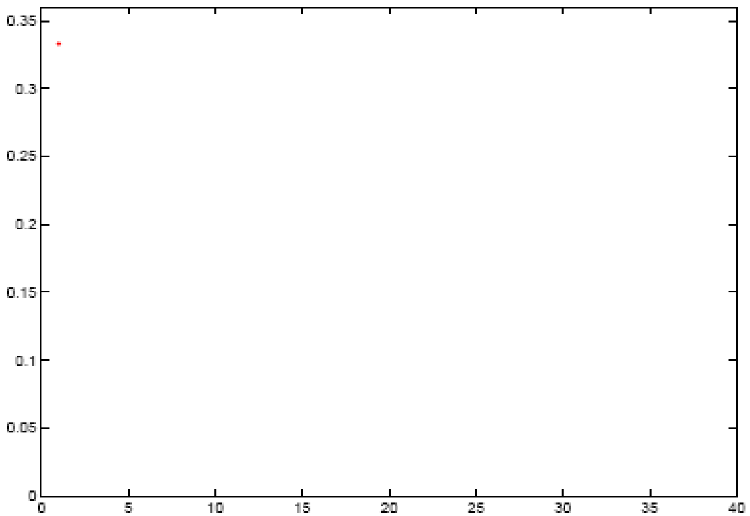
20 iterations



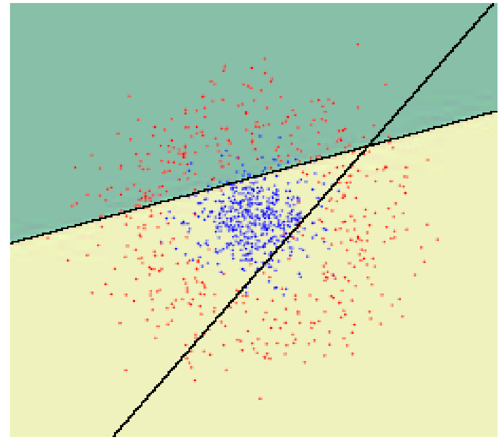
from Elder, John. From Trees to Forests and Rule Sets - A Unified Overview of Ensemble Methods. 2007.

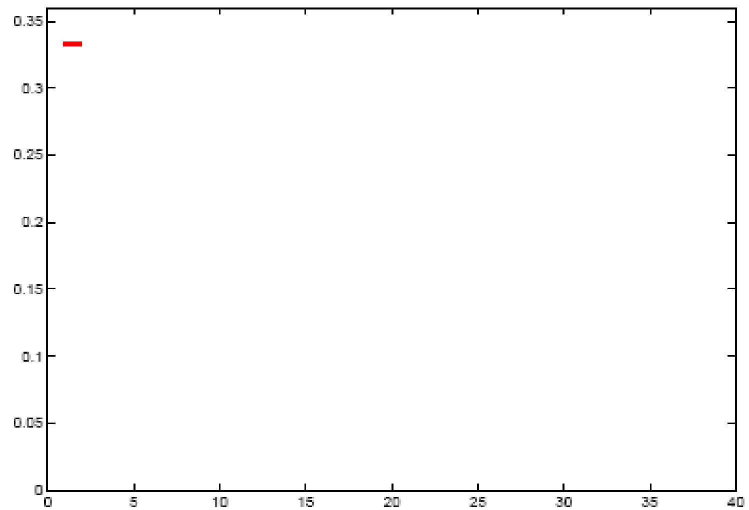
$t = 1$



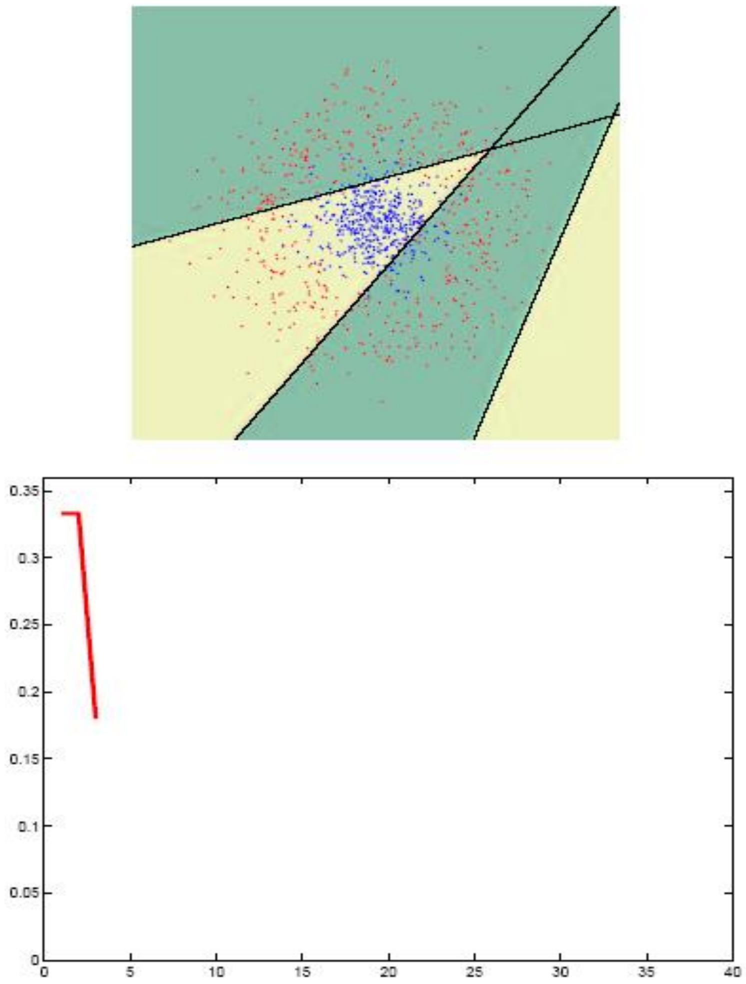

0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
0 5 10 15 20 25 30 35 40

$t = 2$

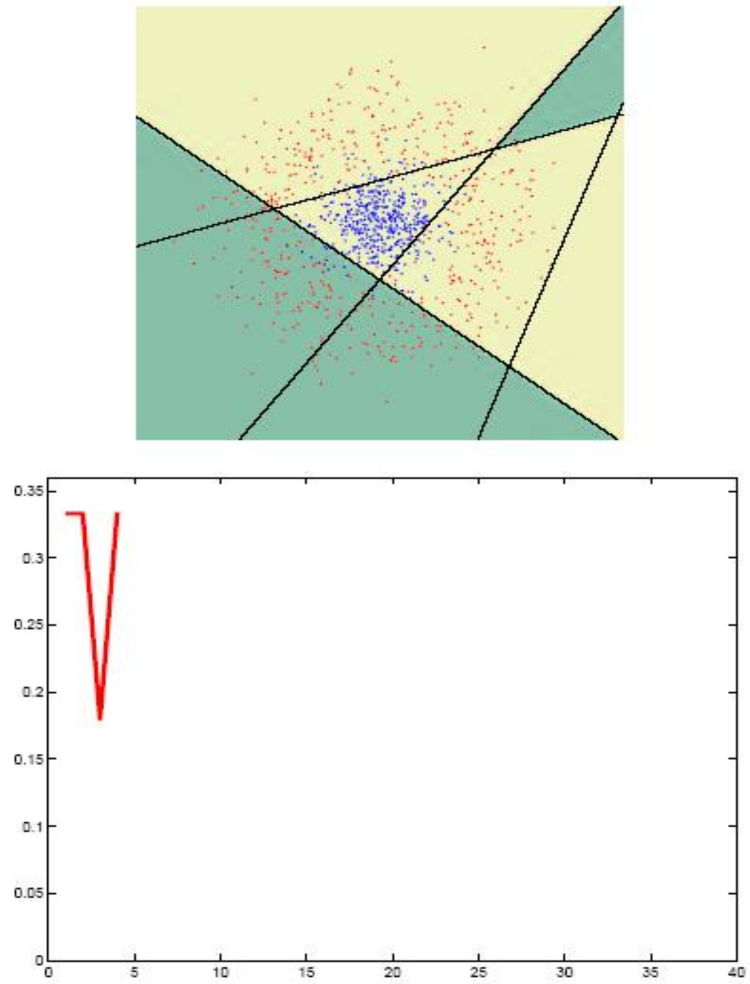



0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
0 5 10 15 20 25 30 35 40

$t = 3$



$t = 4$



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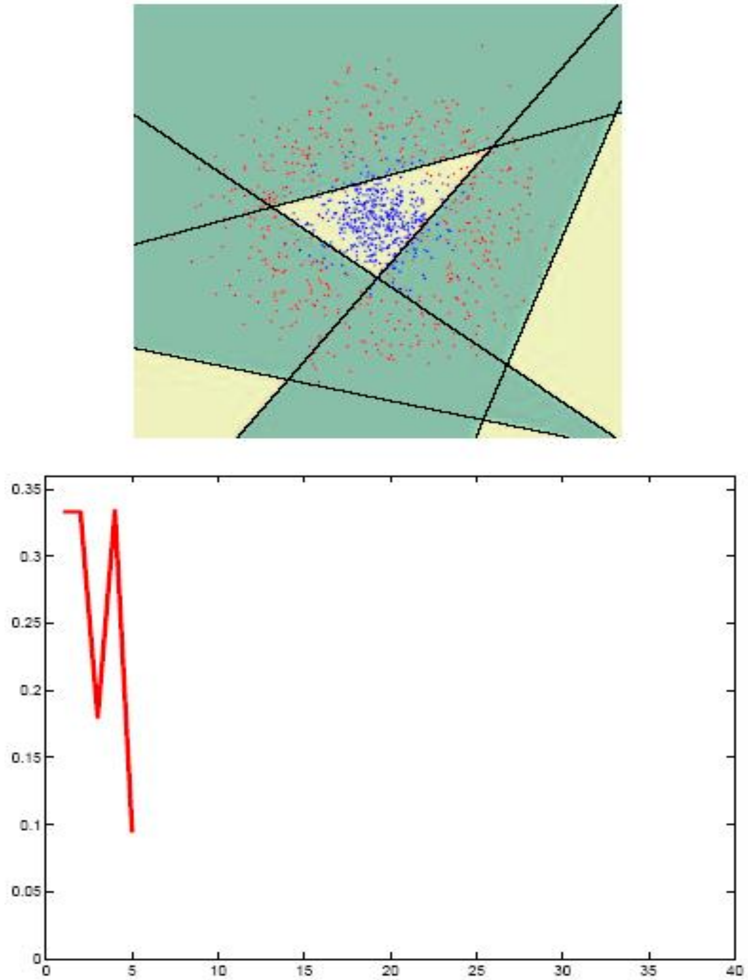
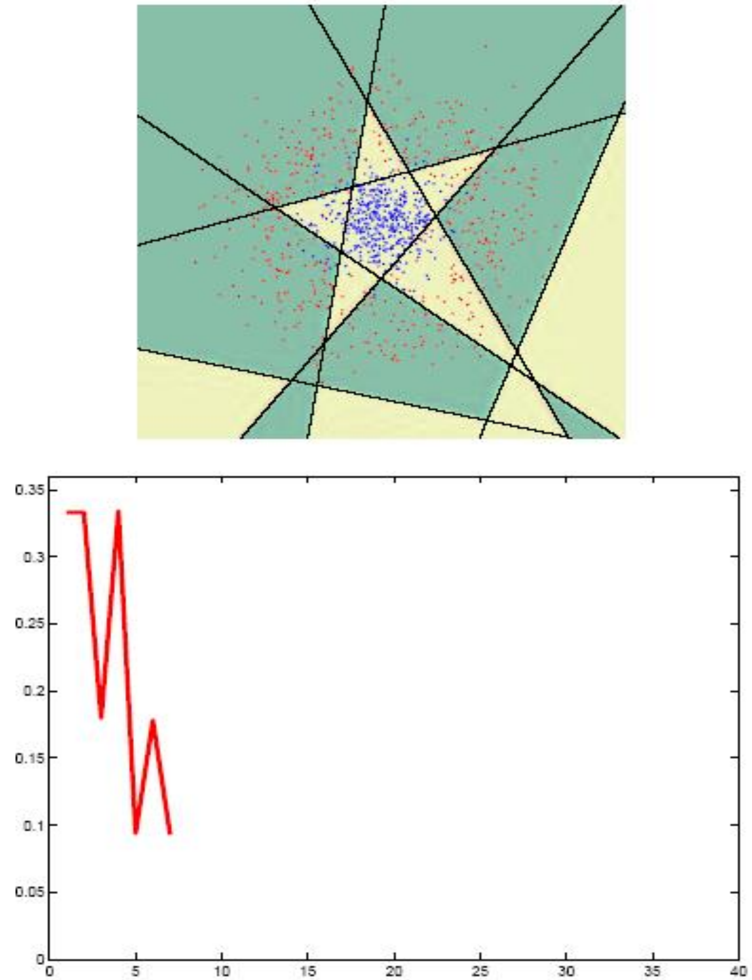
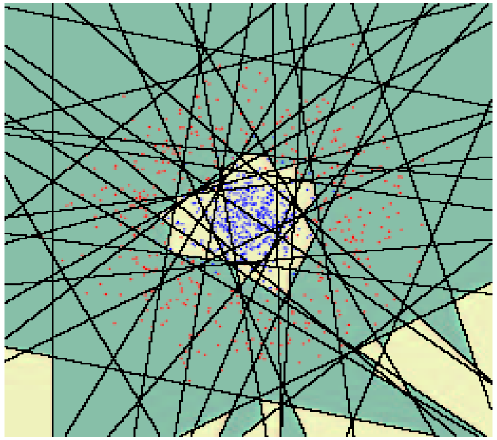
$t = 5$

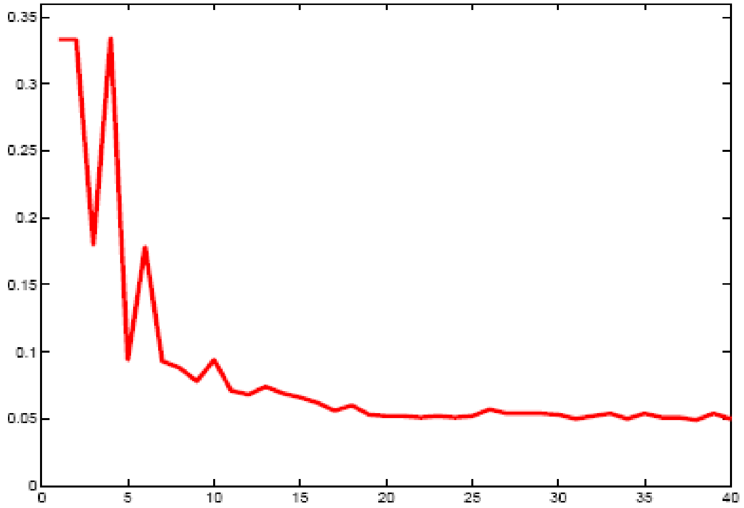

0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
0
5
10
15
20
25
30
35
40

$t = 7$

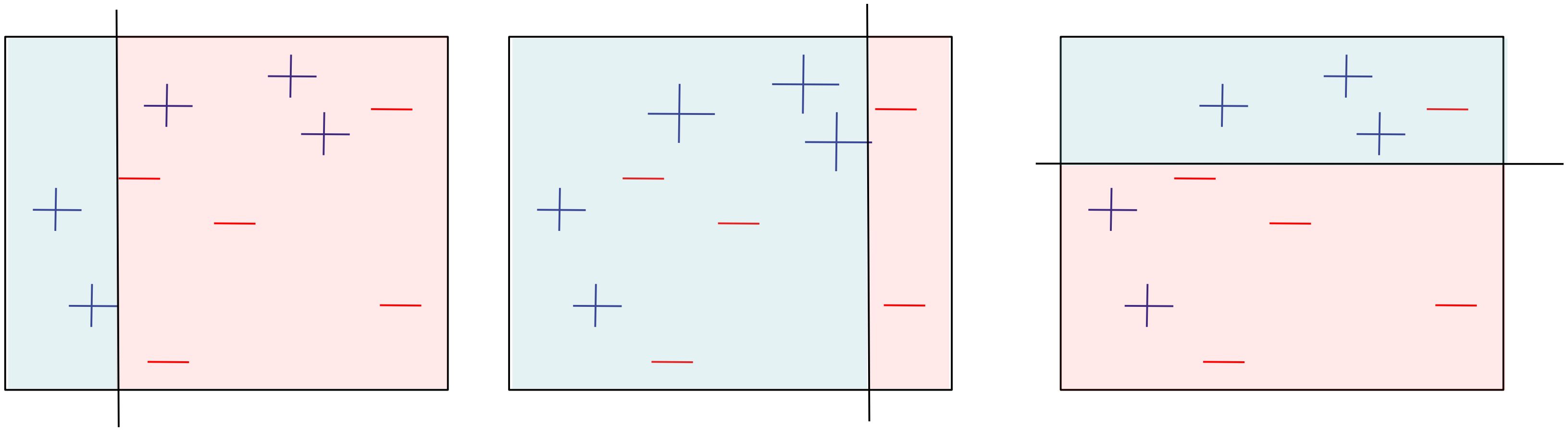

0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
0
5
10
15
20
25
30
35
40

$$t = 40$$

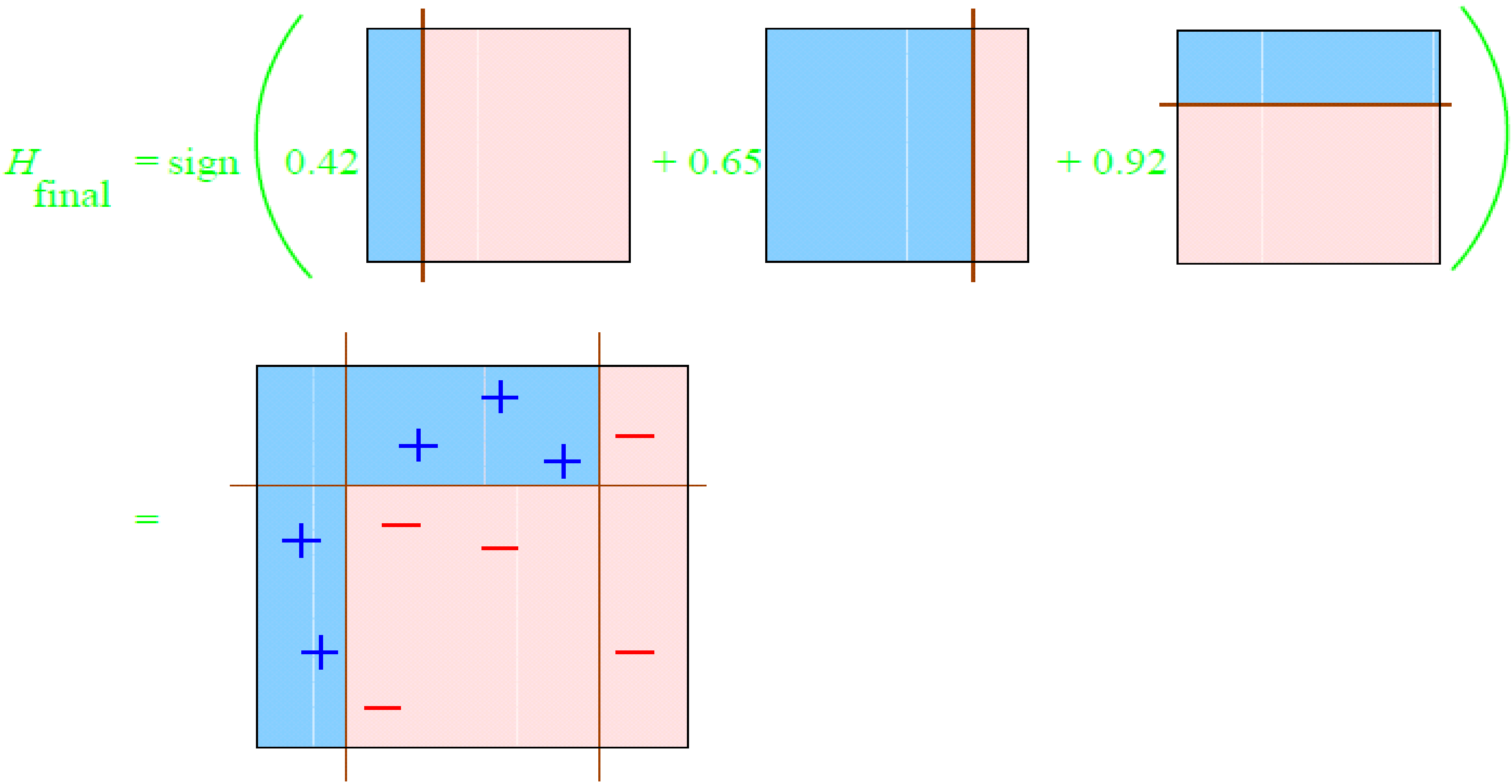




Another Toy Example



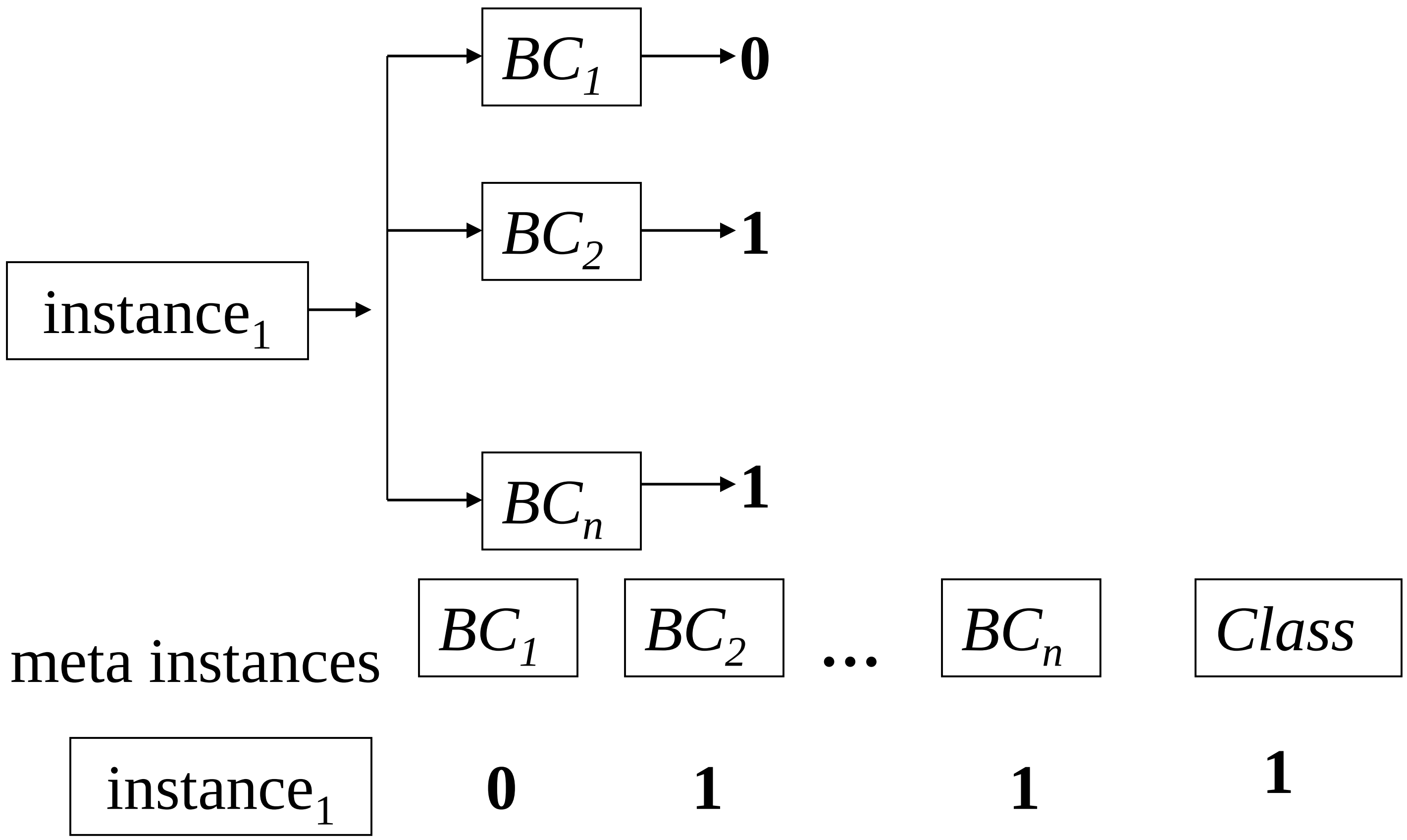
Final Classifier



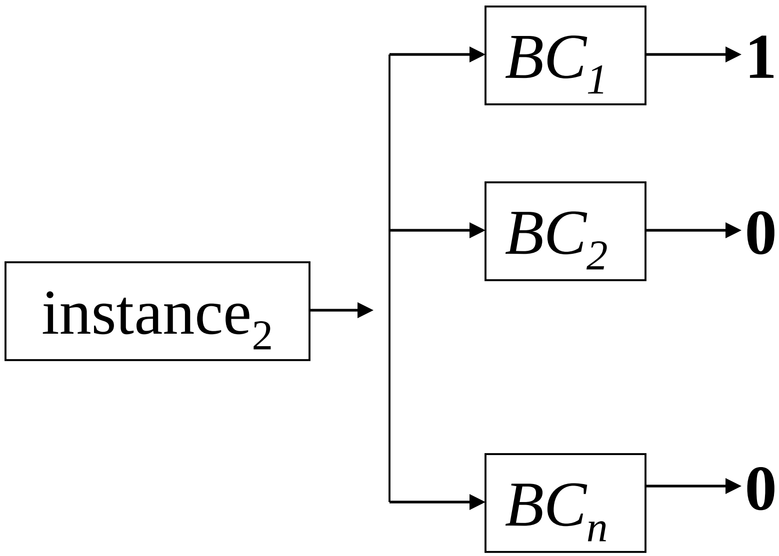
Stacking

- Uses *meta learner* instead of voting to combine predictions of base learners
  - Predictions of base learners (*level-0 models*) are used as input for meta learner (*level-1 model)*
- Base learners usually different learning schemes
- Hard to analyze theoretically: "black magic"

Stacking


$instance_1$
BC_1
0
BC_2
1
BC_n
1
meta instances
BC_1
BC_2
...
BC_n
Class
$instance_1$
0
1
1
1

Stacking



meta instances	BC_1	BC_2	…	BC_n	*Class*
instance$_1$	**0**	**1**		**1**	**1**
instance$_2$	**1**	**0**		**0**	**0**

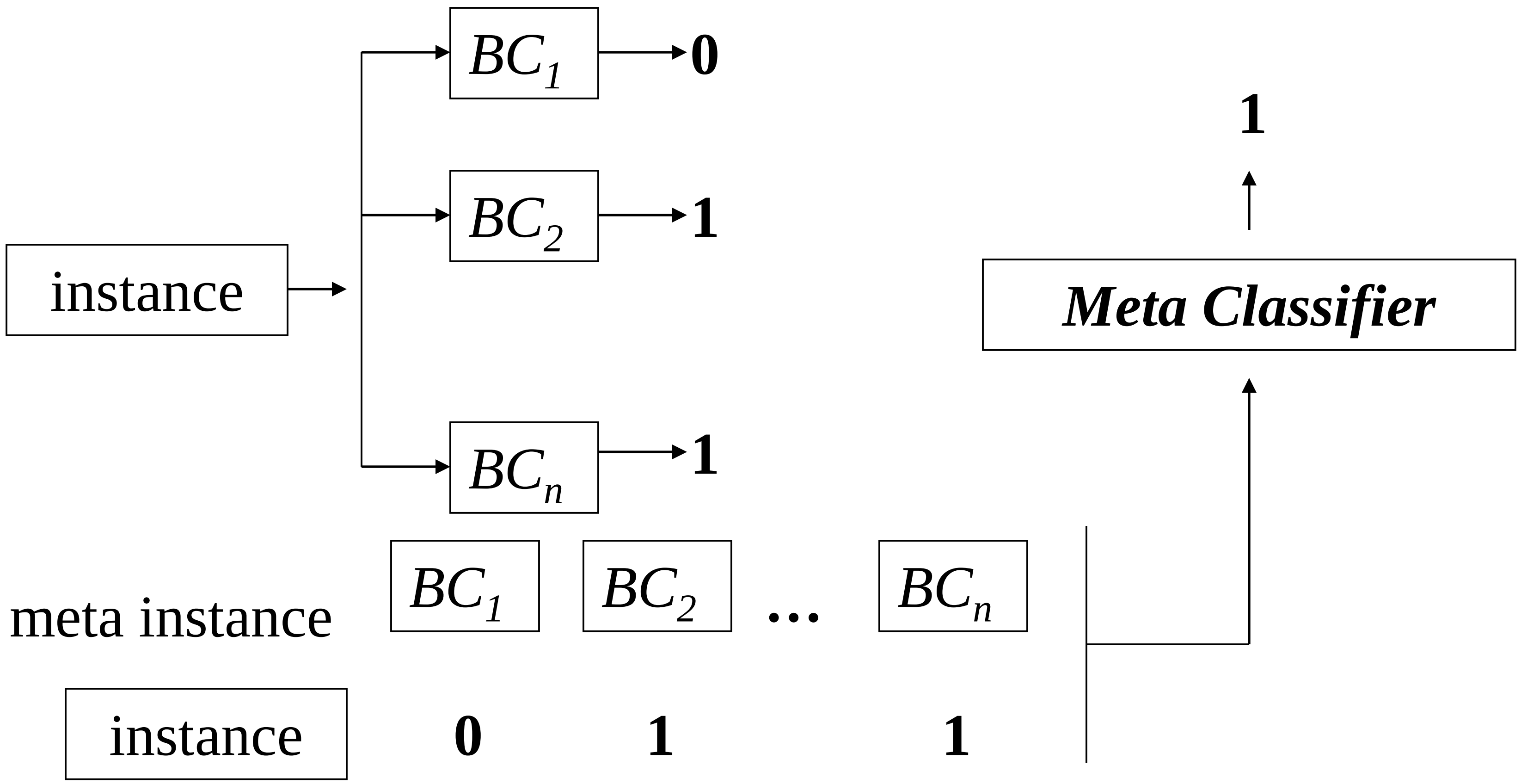
Stacking

Meta Classifier

$\Uparrow$

meta instances	BC_1	BC_2	…	BC_n	*Class*
instance_1	**0**	**1**		**1**	**1**
instance_2	**1**	**0**		**0**	**0**

Stacking



BC1
0
BC2
1
instance
BCn
1
1
Meta Classifier
meta instance
BC1
BC2
...
BCn
instance
0
1
1

More on stacking

- If base learners can output probabilities it's better to use those as input to meta learner
- Which algorithm to use to generate meta learner?
  - In principle, any learning scheme can be applied
  - David Wolpert: "relatively global, smooth" model
    - Base learners do most of the work
    - Reduces risk of overfitting

Outline

- Why ensemble learning?
- Supervised learning
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  - Methods for Coordinated Construction of Ensembles
    - Boosting, Stacking
- **Gradient Boosted Machines**

Gradient Boosting for Regression

Let's play a game...
You are given $(x_1, y_1), (x_2, y_2), ..., (x_n, y_n)$, and the task is to fit a model $F(x)$ to minimize square loss.
Suppose your friend wants to help you and gives you a model F.
You check his model and find the model is good but not perfect.
There are some mistakes: $F(x_1) = 0.8$, while $y_1 = 0.9$, and $F(x_2) = 1.4$ while $y_2 = 1.3$... How can you improve this model?

Rule of the game:

- You are not allowed to remove anything from F or change any parameter in F.
- You can add an additional model (regression tree) h to F, so the new prediction will be $F(x) + h(x)$.

Gradient Boosting for Regression

Simple solution:

You wish to improve the model such that

$$
\begin{aligned}
F(x_1) + h(x_1) &= y_1 \\
F(x_2) + h(x_2) &= y_2 \\
&\dots \\
F(x_n) + h(x_n) &= y_n
\end{aligned}
$$

Or, equivalently, you wish

$$
\begin{aligned}
h(x_1) &= y_1 - F(x_1) \\
h(x_2) &= y_2 - F(x_2) \\
&\dots \\
h(x_n) &= y_n - F(x_n)
\end{aligned}
$$

Just fit a regression tree h to data

$(x_1, y_1 - F(x_1)), (x_2, y_2 - F(x_2)), \dots, (x_n, y_n - F(x_n))$

Gradient Boosting for Regression

$y_i - F(x_i)$ are called **residuals**. These are the parts that existing model F cannot do well.
The role of h is to compensate the shortcoming of existing model F.

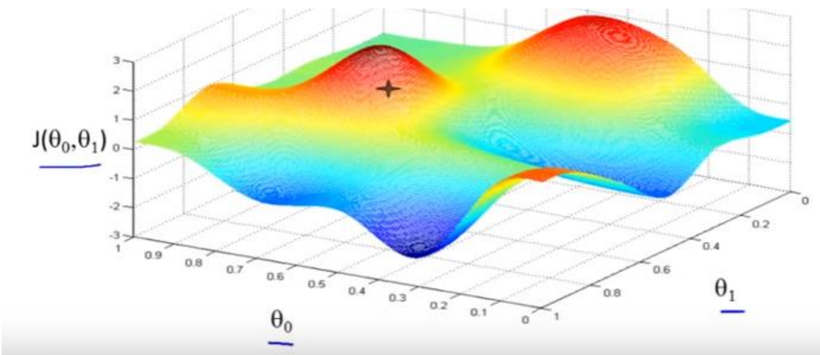
If the new model $F + h$ is still not satisfactory, we can add another regression tree...

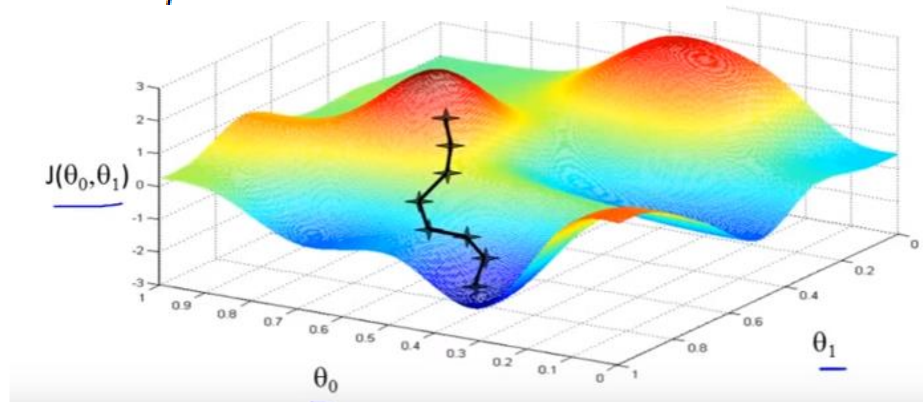
How is this related to gradient descent?

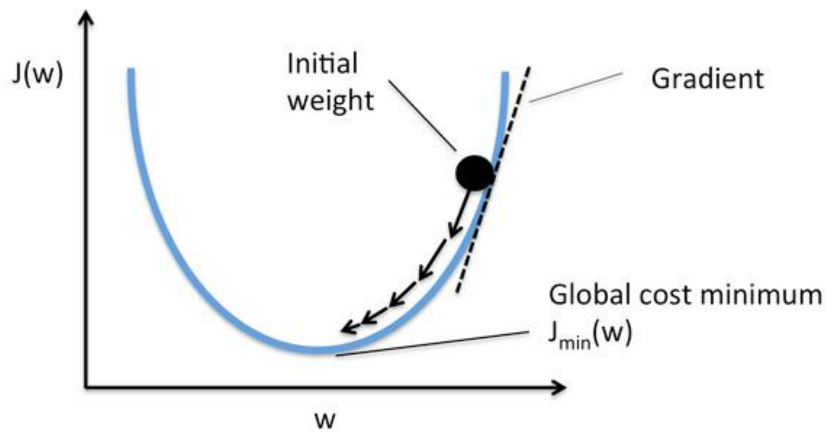
Gradient Descent

Minimize a function by moving in the opposite direction of the gradient.

$$\theta_i := \theta_i - \rho \frac{\partial J}{\partial \theta_i}$$







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Relationship between Gradient descent and GBM

Loss function $L(y, F(x)) = (y - F(x))^2/2$

We want to minimize $J = \sum_i L(y_i, F(x_i))$ by adjusting $F(x_1), F(x_2), ..., F(x_n)$.

$$\frac{\partial J}{\partial F(x_i)} = \frac{\partial \sum_i L(y_i, F(x_i))}{\partial F(x_i)} = \frac{\partial L(y_i, F(x_i))}{\partial F(x_i)} = F(x_i) - y_i$$

So we can interpret residuals as negative gradients.

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

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Relationship between Gradient descent and GBM

$$F(x_i) := F(x_i) + h(x_i)$$
$$F(x_i) := F(x_i) + y_i - F(x_i)$$
$$F(x_i) := F(x_i) - 1\frac{\partial J}{\partial F(x_i)}$$
$$\theta_i := \theta_i - \rho\frac{\partial J}{\partial \theta_i}$$

For regression with **square loss**,

$$\textit{residual} \Leftrightarrow \textit{negative gradient}$$

$$\textit{fit } h \textit{ to residual} \Leftrightarrow \textit{fit } h \textit{ to negative gradient}$$

$$\textit{update } F \textit{ based on residual} \Leftrightarrow \textit{update } F \textit{ based on negative gradient}$$

So we are actually updating our model using **gradient descent**!

It turns out that the concept of **gradients** is more general and useful than the concept of **residuals**.

Regression with square loss

Let us summarize the algorithm we just derived using the concept of gradients. Negative gradient:

$$-g(x_i) = -\frac{\partial L(y_i, F(x_i))}{\partial F(x_i)} = y_i - F(x_i)$$

start with an initial model, say, $F(x) = \frac{\sum_{i=1}^{n} y_i}{n}$
iterate until converge:
  calculate negative gradients $-g(x_i)$
  fit a regression tree h to negative gradients $-g(x_i)$
  $F := F + \rho h$, where $\rho = 1$

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.

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Loss Functions for Regression functions

Why do we need to consider other loss functions? Isn't square loss good enough?

Square loss is:

- ✓ Easy to deal with mathematically
- × Not robust to outliers

  Outliers are heavily punished because the error is squared.

  Example:

y_i	0.5	1.2	2	5*
$F(x_i)$	0.6	1.4	1.5	1.7
$L = (y - F)^2/2$	0.005	0.02	0.125	5.445

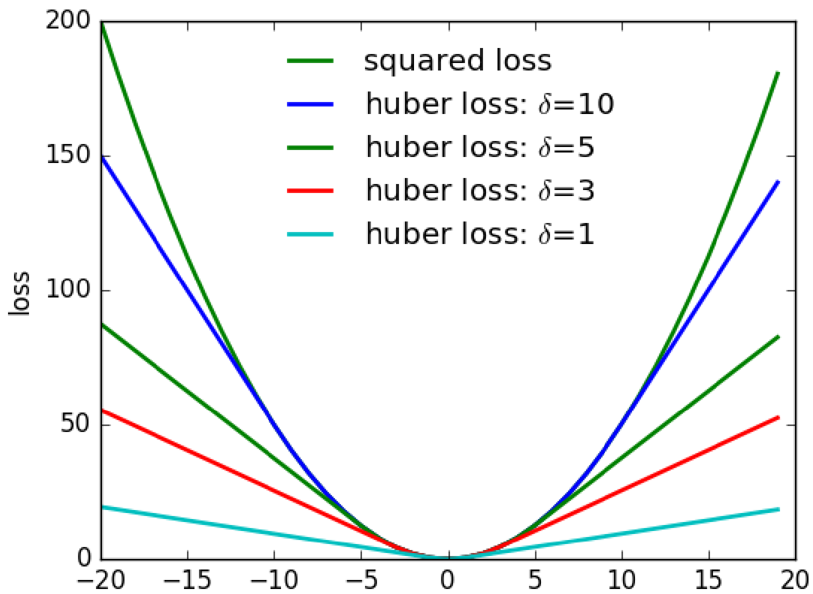
  Consequence?

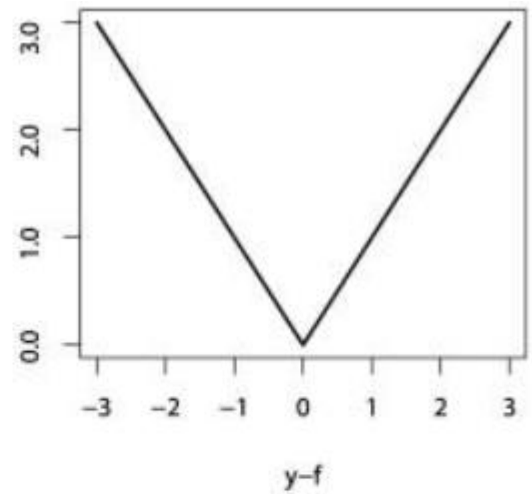
  Pay too much attention to outliers. Try hard to incorporate outliers into the model. Degrade the overall performance.

Loss Functions for Regression functions

- Absolute loss (more robust to outliers)

$$L(y, F) = |y - F|$$





absolute loss function

		1.4	1.5	1.7
		0.02	0.125	5.445
Absolute loss	0.1	0.2	0.5	3.3
Huber loss($\delta = 0.5$)	0.005	0.02	0.125	1.525

Regression with other Loss Functions

Regression with Absolute Loss

Negative gradient:

$$-g(x_i) = -\frac{\partial L(y_i, F(x_i))}{\partial F(x_i)} = sign(y_i - F(x_i))$$

Regression with Huber Loss

Negative gradient:

$$\begin{aligned} -g(x_i) &= -\frac{\partial L(y_i, F(x_i))}{\partial F(x_i)} \\ &= \begin{cases} y_i - F(x_i) & |y_i - F(x_i)| \le \delta \\ \delta sign(y_i - F(x_i)) & |y_i - F(x_i)| > \delta \end{cases} \end{aligned}$$

In general,

$$negative\ gradients \not\Leftrightarrow residuals$$

We should follow negative gradients rather than residuals. Why?

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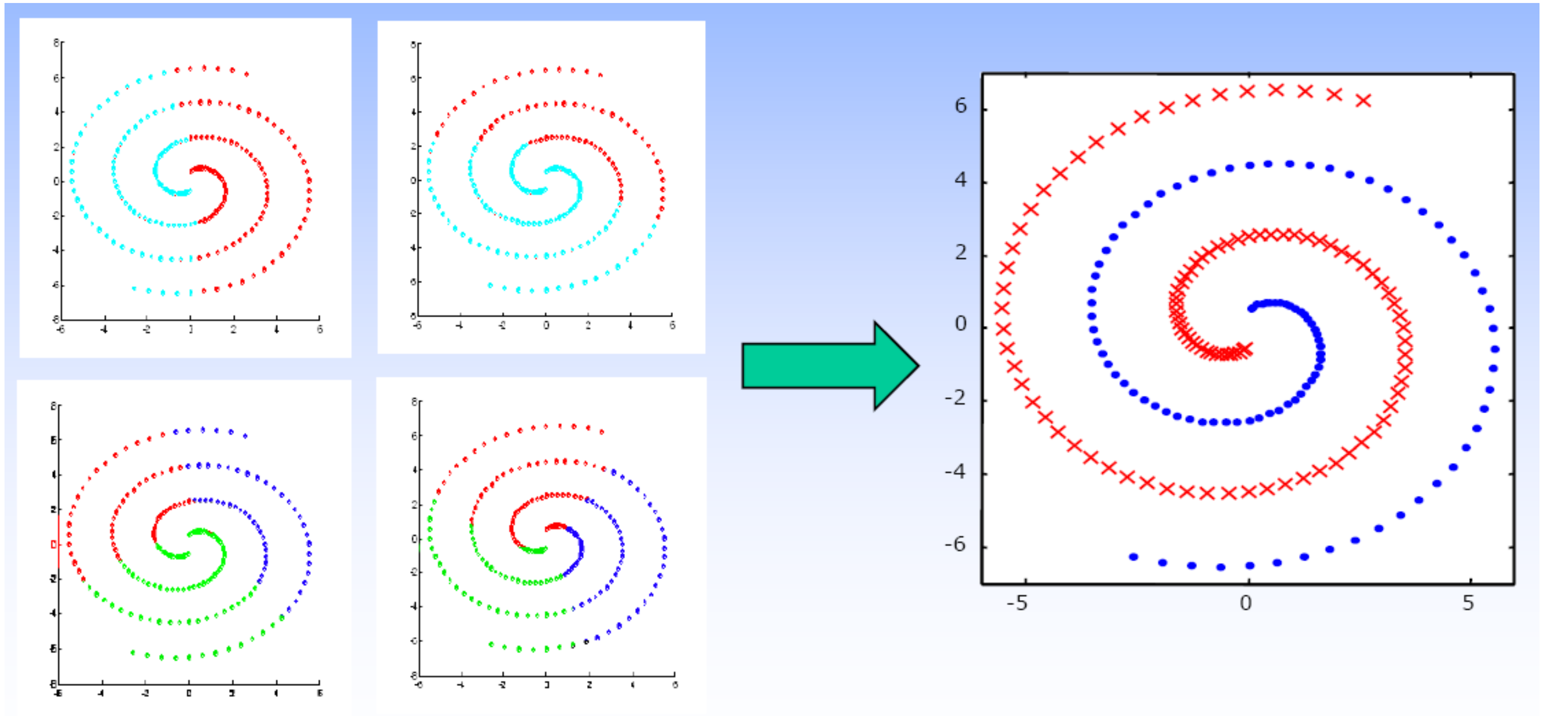
  - Methods for Coordinated Construction of Ensembles
    - Boosting, Stacking
- Gradient Boosted Machines
- **Unsupervised learning**
  - **Clustering ensembles**

Clustering Ensemble

- Problem
  - Given an unlabeled data set $D=\{x_1,x_2,\ldots,x_n\}$
  - An ensemble approach computes:
    - A set of clustering solutions $\{C_1,C_2,\ldots,C_k\}$, each of which maps data to a cluster: $f_j(x)=m$
    - A unified clustering solutions f^* which combines base clustering solutions by their consensus
- Challenges
  - The correspondence between the clusters in different clustering solutions is unknown
  - Unsupervised
  - Combinatorial optimization problem-NP-complete

Motivations

- Goal
  - Combine "weak" clusterings to a better one



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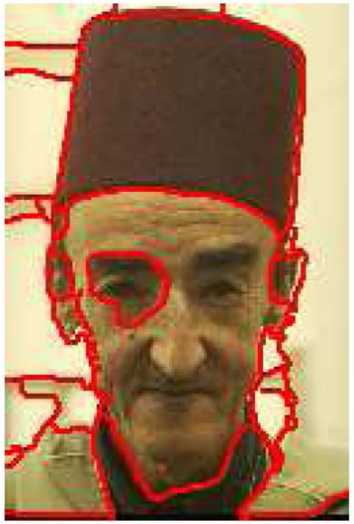
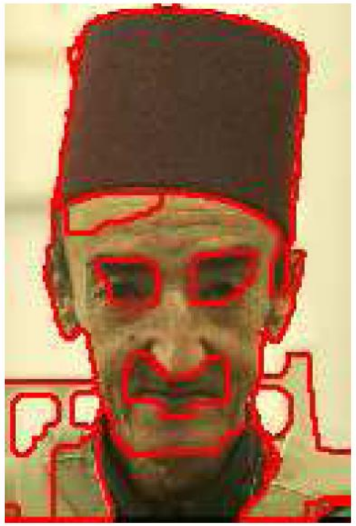
(a)



(b)



(c)

(d)

ensemble

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Take-aways

- Ensembles learning is very useful in obtaining improved models.
- We discussed ensemble learning from two perspectives
  - Supervised ensembles
  - Unsupervised ensembles

Tutorial on Ensemble of Classifiers

- *Survey of Boosting from an Optimization Perspective*. Manfred K. Warmuth and S.V.N. Vishwanathan. ICML'09, Montreal, Canada, June 2009.
- *Theory and Applications of Boosting*. Robert Schapire. NIPS'07, Vancouver, Canada, December 2007.
- *From Trees to Forests and Rule Sets--A Unified Overview of Ensemble Methods*. Giovanni Seni and John Elder. KDD'07, San Jose, CA, August 2007.

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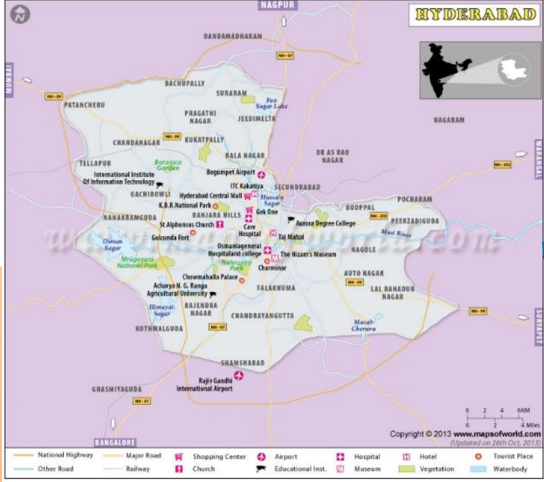

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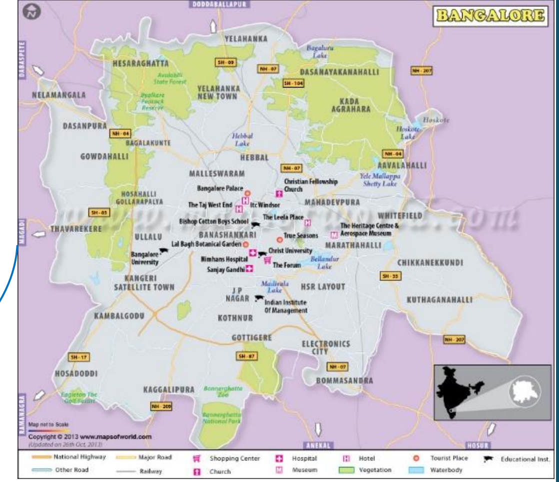

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