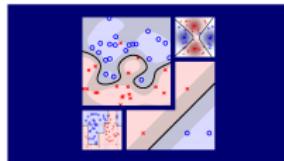


# Machine Learning Techniques (機器學習技法)



Lecture 11: Gradient Boosted Decision Tree

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# Roadmap

- ① Embedding Numerous Features: Kernel Models
- ② Combining Predictive Features: Aggregation Models

## Lecture 10: Random Forest

**bagging of randomized C&RT trees with automatic validation and feature selection**

## Lecture 11: Gradient Boosted Decision Tree

- Adaptive Boosted Decision Tree
- Optimization View of AdaBoost
- Gradient Boosting
- Summary of Aggregation Models

- ③ Distilling Implicit Features: Extraction Models

# From Random Forest to AdaBoost-DTree

function **RandomForest**( $\mathcal{D}$ )

For  $t = 1, 2, \dots, T$

- ➊ request size- $N'$  data  $\tilde{\mathcal{D}}_t$  by bootstrapping with  $\mathcal{D}$
- ➋ obtain tree  $g_t$  by Randomized-DTree( $\tilde{\mathcal{D}}_t$ )

return  $G = \text{Uniform}(\{g_t\})$

function **AdaBoost-DTree**( $\mathcal{D}$ )

For  $t = 1, 2, \dots, T$

- ➊ reweight data by  $\mathbf{u}^{(t)}$
- ➋ obtain tree  $g_t$  by DTree( $\mathcal{D}, \mathbf{u}^{(t)}$ )
- ➌ calculate ‘vote’  $\alpha_t$  of  $g_t$

return  $G = \text{LinearHypo}(\{(g_t, \alpha_t)\})$

need: weighted DTree( $\mathcal{D}, \mathbf{u}^{(t)}$ )

# Weighted Decision Tree Algorithm

## Weighted Algorithm

$$\text{minimize (regularized) } E_{\text{in}}^{\mathbf{u}}(h) = \frac{1}{N} \sum_{n=1}^N \mathbf{u}_n \cdot \text{err}(y_n, h(\mathbf{x}_n))$$

if using existing algorithm as **black box** (no modifications),  
to get  $E_{\text{in}}^{\mathbf{u}}$  approximately optimized.....

### 'Weighted' Algorithm in Bagging

weights  $\mathbf{u}$  expressed by  
bootstrap-sampled copies  
—request size- $N'$  data  $\tilde{\mathcal{D}}_t$   
by bootstrapping with  $\mathcal{D}$

### A General Randomized Base Algorithm

weights  $\mathbf{u}$  expressed by  
sampling proportional to  $\mathbf{u}_n$   
—request size- $N'$  data  $\tilde{\mathcal{D}}_t$   
by sampling  $\propto \mathbf{u}$  on  $\mathcal{D}$

AdaBoost-DTree: often via  
AdaBoost + sampling  $\propto \mathbf{u}^{(t)}$  + DTree( $\tilde{\mathcal{D}}_t$ )  
without modifying DTree

# Weak Decision Tree Algorithm

AdaBoost: **votes**  $\alpha_t = \ln \Delta_t = \ln \sqrt{\frac{1-\epsilon_t}{\epsilon_t}}$  with **weighted error rate**  $\epsilon_t$

if **fully grown** tree trained on **all**  $\mathbf{x}_n$

$\Rightarrow E_{in}(g_t) = 0$  if **all**  $\mathbf{x}_n$  different

$\Rightarrow E_{in}^u(g_t) = 0$

$\Rightarrow \epsilon_t = 0$

$\Rightarrow \alpha_t = \infty$  (**autocracy**!!)

need: **pruned** tree trained on **some**  $\mathbf{x}_n$  to be **weak**

- **pruned**: usual pruning, or just **limiting tree height**
- **some**: **sampling**  $\propto \mathbf{u}^{(t)}$

AdaBoost-DTree: often via AdaBoost +  
**sampling**  $\propto \mathbf{u}^{(t)}$  + **pruned** DTree( $\tilde{\mathcal{D}}$ )

# AdaBoost with Extremely-Pruned Tree

what if DTree with **height**  $\leq 1$  (extremely pruned)?

DTree (C&RT) with **height**  $\leq 1$

learn **branching criteria**

$$b(\mathbf{x}) = \underset{\text{decision stumps } h(\mathbf{x})}{\operatorname{argmin}} \sum_{c=1}^2 |\mathcal{D}_c \text{ with } h| \cdot \text{impurity}(\mathcal{D}_c \text{ with } h)$$

—if **impurity** = binary classification error,

**just a decision stump, remember? :-)**

**AdaBoost-Stump**  
= **special case** of AdaBoost-DTree

## Fun Time

When running AdaBoost-DTree with sampling and getting a decision tree  $g_t$  such that  $g_t$  achieves zero error on the sampled data set  $\tilde{D}_t$ . Which of the following is possible?

- 1  $\alpha_t < 0$
- 2  $\alpha_t = 0$
- 3  $\alpha_t > 0$
- 4 all of the above

## Fun Time

When running AdaBoost-DTree with sampling and getting a decision tree  $g_t$  such that  $g_t$  achieves zero error on the sampled data set  $\tilde{D}_t$ . Which of the following is possible?

- 1  $\alpha_t < 0$
- 2  $\alpha_t = 0$
- 3  $\alpha_t > 0$
- 4 all of the above

Reference Answer: ④

While  $g_t$  achieves zero error on  $\tilde{D}_t$ ,  $g_t$  may not achieve zero weighted error on  $(\mathcal{D}, \mathbf{u}^{(t)})$  and hence  $\epsilon_t$  can be anything, even  $\geq \frac{1}{2}$ . Then,  $\alpha_t$  can be  $\leq 0$ .

# Example Weights of AdaBoost

$$u_n^{(t+1)} = \begin{cases} u_n^{(t)} \cdot \diamond_t & \text{if incorrect} \\ u_n^{(t)}/\diamond_t & \text{if correct} \end{cases}$$

$$= u_n^{(t)} \cdot \diamond_t^{-y_n g_t(\mathbf{x}_n)} = u_n^{(t)} \cdot \exp(-y_n \alpha_t g_t(\mathbf{x}_n))$$

$$u_n^{(T+1)} = u_n^{(1)} \cdot \prod_{t=1}^T \exp(-y_n \alpha_t g_t(\mathbf{x}_n)) = \frac{1}{N} \cdot \exp \left( -y_n \sum_{t=1}^T \alpha_t g_t(\mathbf{x}_n) \right)$$

- recall:  $G(\mathbf{x}) = \text{sign} \left( \sum_{t=1}^T \alpha_t g_t(\mathbf{x}) \right)$
- $\sum_{t=1}^T \alpha_t g_t(\mathbf{x})$ : **voting score** of  $\{g_t\}$  on  $\mathbf{x}$

AdaBoost:  $u_n^{(T+1)} \propto \exp(-y_n (\text{voting score on } \mathbf{x}_n))$

# Voting Score and Margin

linear blending = LinModel + hypotheses as transform + ~~constraints~~

$$G(\mathbf{x}_n) = \text{sign} \left( \sum_{t=1}^T \underbrace{\alpha_t}_{w_i} \underbrace{g_t(\mathbf{x}_n)}_{\phi_i(\mathbf{x}_n)} \right)$$

and hard-margin SVM margin =  $\frac{y_n \cdot (\mathbf{w}^T \phi(\mathbf{x}_n) + b)}{\|\mathbf{w}\|}$ , remember? :-)

$y_n(\text{voting score})$  = signed & unnormalized margin

want  $y_n(\text{voting score})$  positive & large

$\Leftrightarrow \exp(-y_n(\text{voting score}))$  small

$\Leftrightarrow u_n^{(T+1)}$  small

claim: AdaBoost decreases  $\sum_{n=1}^N u_n^{(t)}$

# AdaBoost Error Function

claim: AdaBoost **decreases**  $\sum_{n=1}^N u_n^{(t)}$  and thus somewhat **minimizes**

$$\sum_{n=1}^N u_n^{(T+1)} = \frac{1}{N} \sum_{n=1}^N \exp \left( -y_n \sum_{t=1}^T \alpha_t g_t(\mathbf{x}_n) \right)$$

linear score  $s = \sum_{t=1}^T \alpha_t g_t(\mathbf{x}_n)$

- $\text{err}_{0/1}(s, y) = \llbracket ys \leq 0 \rrbracket$
- $\widehat{\text{err}}_{\text{ADA}}(s, y) = \exp(-ys)$ :  
upper bound of  $\text{err}_{0/1}$   
—called **exponential error measure**

$\widehat{\text{err}}_{\text{ADA}}$ : **algorithmic error measure**  
by **convex upper bound** of  $\text{err}_{0/1}$

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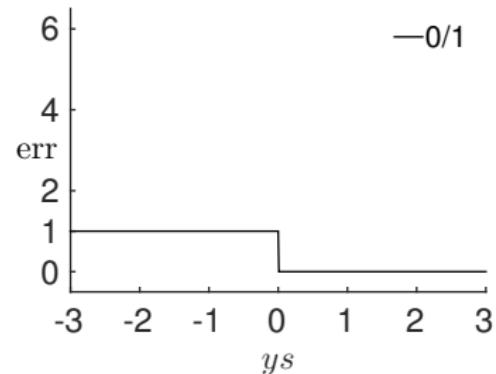
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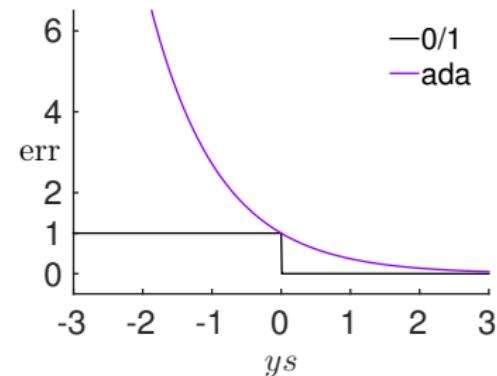
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$\widehat{\text{err}}_{\text{ADA}}$ : **algorithmic error measure**  
by **convex upper bound** of  $\text{err}_{0/1}$

# Gradient Descent on AdaBoost Error Function

recall: gradient descent (**remember? :-)**), at iteration  $t$

$$\min_{\|\mathbf{v}\|=1} E_{\text{in}}(\mathbf{w}_t + \eta \mathbf{v}) \approx \underbrace{E_{\text{in}}(\mathbf{w}_t)}_{\text{known}} + \underbrace{\eta}_{\text{given positive}} \underbrace{\mathbf{v}^T \nabla E_{\text{in}}(\mathbf{w}_t)}_{\text{known}}$$

at iteration  $t$ , to find  $g_t$ , solve

$$\begin{aligned} \min_h \hat{E}_{\text{ADA}} &= \frac{1}{N} \sum_{n=1}^N \exp \left( -y_n \left( \sum_{\tau=1}^{t-1} \alpha_\tau g_\tau(\mathbf{x}_n) + \eta h(\mathbf{x}_n) \right) \right) \\ &= \sum_{n=1}^N u_n^{(t)} \exp (-y_n \eta h(\mathbf{x}_n)) \\ \underset{\text{taylor}}{\approx} \sum_{n=1}^N u_n^{(t)} (1 - y_n \eta h(\mathbf{x}_n)) &= \sum_{n=1}^N u_n^{(t)} - \eta \sum_{n=1}^N u_n^{(t)} y_n h(\mathbf{x}_n) \end{aligned}$$

good  $h$ : minimize  $\sum_{n=1}^N u_n^{(t)} (-y_n h(\mathbf{x}_n))$

# Learning Hypothesis as Optimization

finding good  $h$  (function direction)  $\Leftrightarrow$  minimize  $\sum_{n=1}^N u_n^{(t)} (-y_n h(\mathbf{x}_n))$

for binary classification, where  $y_n$  and  $h(\mathbf{x}_n)$  both  $\in \{-1, +1\}$ :

$$\begin{aligned}\sum_{n=1}^N u_n^{(t)} (-y_n h(\mathbf{x}_n)) &= \sum_{n=1}^N u_n^{(t)} \left\{ \begin{array}{ll} -1 & \text{if } y_n = h(\mathbf{x}_n) \\ +1 & \text{if } y_n \neq h(\mathbf{x}_n) \end{array} \right. \\ &= - \sum_{n=1}^N u_n^{(t)} + \sum_{n=1}^N u_n^{(t)} \left\{ \begin{array}{ll} 0 & \text{if } y_n = h(\mathbf{x}_n) \\ 2 & \text{if } y_n \neq h(\mathbf{x}_n) \end{array} \right. \\ &= - \sum_{n=1}^N u_n^{(t)} + 2E_{\text{in}}^{u^{(t)}}(h) \cdot N\end{aligned}$$

—who minimizes  $E_{\text{in}}^{u^{(t)}}(h)$ ? **A in AdaBoost! :-)**

**A:** **good**  $g_t = h$  for ‘gradient descent’

# Deciding Blending Weight as Optimization

AdaBoost finds  $g_t$  by approximately  $\min_h \widehat{E}_{\text{ADA}} = \sum_{n=1}^N u_n^{(t)} \exp(-y_n \eta h(\mathbf{x}_n))$

after finding  $g_t$ , how about

$$\min_{\eta} \widehat{E}_{\text{ADA}} = \sum_{n=1}^N u_n^{(t)} \exp(-y_n \eta g_t(\mathbf{x}_n))$$

- optimal  $\eta_t$  somewhat '**greedily faster**' than fixed (small)  $\eta$   
—called **steepest** descent for optimization
- two cases inside summation:
  - $y_n = g_t(\mathbf{x}_n)$  :  $u_n^{(t)} \exp(-\eta)$  (correct)
  - $y_n \neq g_t(\mathbf{x}_n)$  :  $u_n^{(t)} \exp(+\eta)$  (incorrect)
- $\widehat{E}_{\text{ADA}} = \left( \sum_{n=1}^N u_n^{(t)} \right) \cdot \left( (1 - \epsilon_t) \exp(-\eta) + \epsilon_t \exp(+\eta) \right)$

by solving  $\frac{\partial \widehat{E}_{\text{ADA}}}{\partial \eta} = 0$ , **steepest**  $\eta_t = \ln \sqrt{\frac{1-\epsilon_t}{\epsilon_t}} = \alpha_t$ , **remember? :-)**  
—AdaBoost: **steepest** descent with **approximate functional gradient**

# Fun Time

With  $\widehat{E}_{\text{ADA}} = \left( \sum_{n=1}^N u_n^{(t)} \right) \cdot \left( (1 - \epsilon_t) \exp(-\eta) + \epsilon_t \exp(+\eta) \right)$ , which of the following is  $\frac{\partial \widehat{E}_{\text{ADA}}}{\partial \eta}$  that can be used for solving the optimal  $\eta_t$ ?

- ①  $\left( \sum_{n=1}^N u_n^{(t)} \right) \cdot \left( + (1 - \epsilon_t) \exp(-\eta) + \epsilon_t \exp(+\eta) \right)$
- ②  $\left( \sum_{n=1}^N u_n^{(t)} \right) \cdot \left( + (1 - \epsilon_t) \exp(-\eta) - \epsilon_t \exp(+\eta) \right)$
- ③  $\left( \sum_{n=1}^N u_n^{(t)} \right) \cdot \left( - (1 - \epsilon_t) \exp(-\eta) + \epsilon_t \exp(+\eta) \right)$
- ④  $\left( \sum_{n=1}^N u_n^{(t)} \right) \cdot \left( - (1 - \epsilon_t) \exp(-\eta) - \epsilon_t \exp(+\eta) \right)$

# Fun Time

With  $\widehat{E}_{\text{ADA}} = \left( \sum_{n=1}^N u_n^{(t)} \right) \cdot \left( (1 - \epsilon_t) \exp(-\eta) + \epsilon_t \exp(+\eta) \right)$ , which of the following is  $\frac{\partial \widehat{E}_{\text{ADA}}}{\partial \eta}$  that can be used for solving the optimal  $\eta_t$ ?

- ①  $\left( \sum_{n=1}^N u_n^{(t)} \right) \cdot \left( + (1 - \epsilon_t) \exp(-\eta) + \epsilon_t \exp(+\eta) \right)$
- ②  $\left( \sum_{n=1}^N u_n^{(t)} \right) \cdot \left( + (1 - \epsilon_t) \exp(-\eta) - \epsilon_t \exp(+\eta) \right)$
- ③  $\left( \sum_{n=1}^N u_n^{(t)} \right) \cdot \left( - (1 - \epsilon_t) \exp(-\eta) + \epsilon_t \exp(+\eta) \right)$
- ④  $\left( \sum_{n=1}^N u_n^{(t)} \right) \cdot \left( - (1 - \epsilon_t) \exp(-\eta) - \epsilon_t \exp(+\eta) \right)$

Reference Answer: ③

Differentiate  $\exp(-\eta)$  and  $\exp(+\eta)$  with respect to  $\eta$  and you should easily get the result.

# Gradient Boosting for Arbitrary Error Function

## AdaBoost

$$\min_{\eta} \min_h \frac{1}{N} \sum_{n=1}^N \exp \left( -y_n \left( \sum_{\tau=1}^{t-1} \alpha_\tau g_\tau(\mathbf{x}_n) + \eta h(\mathbf{x}_n) \right) \right)$$

with binary-output hypothesis  $h$

## GradientBoost

$$\min_{\eta} \min_h \frac{1}{N} \sum_{n=1}^N \text{err} \left( \sum_{\tau=1}^{t-1} \alpha_\tau g_\tau(\mathbf{x}_n) + \eta h(\mathbf{x}_n), y_n \right)$$

with any hypothesis  $h$  (usually real-output hypothesis)

GradientBoost: allows **extension to different err** for regression/soft classification/etc.

# GradientBoost for Regression

$$\min_{\eta} \min_h \frac{1}{N} \sum_{n=1}^N \text{err}\left(\underbrace{\sum_{\tau=1}^{t-1} \alpha_\tau g_\tau(\mathbf{x}_n) + \eta h(\mathbf{x}_n)}_{s_n}, y_n\right) \text{ with } \text{err}(s, y) = (s - y)^2$$

$$\begin{aligned} \min_h \dots & \stackrel{\text{taylor}}{\approx} \min_h \quad \frac{1}{N} \sum_{n=1}^N \underbrace{\text{err}(s_n, y_n)}_{\text{constant}} + \frac{1}{N} \sum_{n=1}^N \eta h(\mathbf{x}_n) \left. \frac{\partial \text{err}(s, y_n)}{\partial s} \right|_{s=s_n} \\ &= \min_h \quad \text{constants} + \frac{\eta}{N} \sum_{n=1}^N h(\mathbf{x}_n) \cdot 2(s_n - y_n) \end{aligned}$$

naïve solution  $h(\mathbf{x}_n) = -\infty \cdot (s_n - y_n)$   
if no constraint on  $h$

# Learning Hypothesis as Optimization

$$\min_h \text{ constants} + \frac{\eta}{N} \sum_{n=1}^N 2h(\mathbf{x}_n)(s_n - y_n)$$

- magnitude of  $h$  does not matter: because  $\eta$  will be optimized next
- penalize large magnitude to avoid naïve solution

$$\begin{aligned} \min_h & \quad \text{constants} + \frac{\eta}{N} \sum_{n=1}^N (2h(\mathbf{x}_n)(s_n - y_n) + (h(\mathbf{x}_n))^2) \\ & = \text{constants} + \frac{\eta}{N} \sum_{n=1}^N \left( \text{constant} + (h(\mathbf{x}_n) - (y_n - s_n))^2 \right) \end{aligned}$$

- solution of **penalized approximate functional gradient**: squared-error regression on  $\{(x_n, \underbrace{y_n - s_n}_{\text{residual}})\}$

GradientBoost for regression:

find  $g_t = h$  by regression with **residuals**

# Deciding Blending Weight as Optimization

after finding  $g_t = h$ ,

$$\min_{\eta} \min_h \frac{1}{N} \sum_{n=1}^N \text{err}\left(\underbrace{\sum_{\tau=1}^{t-1} \alpha_\tau g_\tau(\mathbf{x}_n) + \eta g_t(\mathbf{x}_n)}_{s_n}, y_n\right) \text{ with } \text{err}(s, y) = (s - y)^2$$

$$\min_{\eta} \frac{1}{N} \sum_{n=1}^N (s_n + \eta g_t(\mathbf{x}_n) - y_n)^2 = \frac{1}{N} \sum_{n=1}^N ((y_n - s_n) - \eta g_t(\mathbf{x}_n))^2$$

— one-variable linear regression on  $\{(g_t\text{-transformed input, residual})\}$

GradientBoost for regression:  $\alpha_t = \text{optimal } \eta$   
by  $g_t$ -transformed linear regression

# Putting Everything Together

## Gradient Boosted Decision Tree (GBDT)

$$s_1 = s_2 = \dots = s_N = 0$$

for  $t = 1, 2, \dots, T$

- ① obtain  $g_t$  by  $\mathcal{A}(\{(x_n, y_n - s_n)\})$  where  $\mathcal{A}$  is a (squared-error) regression algorithm  
—**how about sampled and pruned C&RT?**

- ② compute  $\alpha_t = \text{OneVarLinearRegression}(\{(g_t(x_n), y_n - s_n)\})$
- ③ update  $s_n \leftarrow s_n + \alpha_t g_t(x_n)$

return  $G(\mathbf{x}) = \sum_{t=1}^T \alpha_t g_t(\mathbf{x})$

**GBDT**: ‘regression sibling’ of AdaBoost-DTree  
—**popular in practice**

# Fun Time

Which of the following is the optimal  $\eta$  for

$$\min_{\eta} \quad \frac{1}{N} \sum_{n=1}^N ((y_n - s_n) - \eta g_t(\mathbf{x}_n))^2$$

- ①  $(\sum_{n=1}^N g_t(\mathbf{x}_n)(y_n - s_n)) \cdot (\sum_{n=1}^N g_t^2(\mathbf{x}_n))$
- ②  $(\sum_{n=1}^N g_t(\mathbf{x}_n)(y_n - s_n)) / (\sum_{n=1}^N g_t^2(\mathbf{x}_n))$
- ③  $(\sum_{n=1}^N g_t(\mathbf{x}_n)(y_n - s_n)) + (\sum_{n=1}^N g_t^2(\mathbf{x}_n))$
- ④  $(\sum_{n=1}^N g_t(\mathbf{x}_n)(y_n - s_n)) - (\sum_{n=1}^N g_t^2(\mathbf{x}_n))$

# Fun Time

Which of the following is the optimal  $\eta$  for

$$\min_{\eta} \quad \frac{1}{N} \sum_{n=1}^N ((y_n - s_n) - \eta g_t(\mathbf{x}_n))^2$$

- ①  $(\sum_{n=1}^N g_t(\mathbf{x}_n)(y_n - s_n)) \cdot (\sum_{n=1}^N g_t^2(\mathbf{x}_n))$
- ②  $(\sum_{n=1}^N g_t(\mathbf{x}_n)(y_n - s_n)) / (\sum_{n=1}^N g_t^2(\mathbf{x}_n))$
- ③  $(\sum_{n=1}^N g_t(\mathbf{x}_n)(y_n - s_n)) + (\sum_{n=1}^N g_t^2(\mathbf{x}_n))$
- ④  $(\sum_{n=1}^N g_t(\mathbf{x}_n)(y_n - s_n)) - (\sum_{n=1}^N g_t^2(\mathbf{x}_n))$

Reference Answer: ②

Derived within Lecture 9 of ML Foundations,  
**remember? :-)**

# Map of Blending Models

blending: aggregate **after getting diverse  $g_t$**

uniform

simple  
voting/averaging of  $g_t$

non-uniform

linear model on  
 $g_t$ -transformed inputs

conditional

nonlinear model on  
 $g_t$ -transformed inputs

uniform for ‘stability’;  
non-uniform/conditional **carefully** for  
‘complexity’

# Map of Aggregation-Learning Models

learning: aggregate **as well as getting diverse  $g_t$**

## Bagging

diverse  $g_t$  by  
bootstrapping;  
uniform vote  
by nothing :-)

## AdaBoost

diverse  $g_t$   
by reweighting;  
linear vote  
by steepest search

## Decision Tree

diverse  $g_t$   
by data splitting;  
conditional vote  
by branching

## GradientBoost

diverse  $g_t$   
by residual fitting;  
linear vote  
by steepest search

**boosting-like algorithms** most popular

# Map of Aggregation of Aggregation Models

Bagging

Random Forest

randomized bagging  
+ 'strong' DTree

AdaBoost

AdaBoost-DTree

AdaBoost  
+ 'weak' DTree

Decision Tree

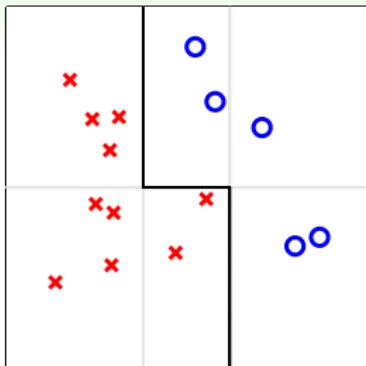
GradientBoost

GBDT

GradientBoost  
+ 'weak' DTree

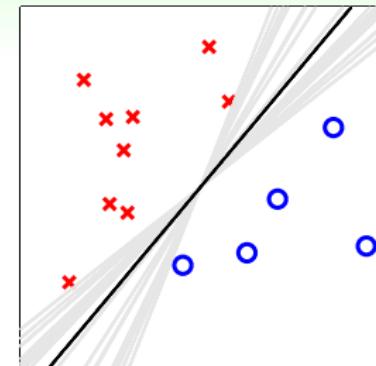
**all three** frequently used in practice

# Specialty of Aggregation Models



cure underfitting

- $G(\mathbf{x})$  ‘strong’
- aggregation  
⇒ **feature transform**



cure overfitting

- $G(\mathbf{x})$  ‘moderate’
- aggregation  
⇒ **regularization**

proper aggregation (a.k.a. ‘ensemble’)  
⇒ **better performance**

## Fun Time

Which of the following aggregation model learns diverse  $g_t$  by reweighting and calculates linear vote by steepest search?

- ① AdaBoost
- ② Random Forest
- ③ Decision Tree
- ④ Linear Blending

## Fun Time

Which of the following aggregation model learns diverse  $g_t$  by reweighting and calculates linear vote by steepest search?

- ① AdaBoost
- ② Random Forest
- ③ Decision Tree
- ④ Linear Blending

Reference Answer: ①

Congratulations on being an expert in aggregation models! :-)

# Summary

- ① Embedding Numerous Features: Kernel Models
- ② Combining Predictive Features: Aggregation Models

## Lecture 11: Gradient Boosted Decision Tree

- Adaptive Boosted Decision Tree
  - sampling and pruning for ‘weak’ trees**
- Optimization View of AdaBoost
  - functional gradient descent on exponential error**
- Gradient Boosting
  - iterative steepest residual fitting**
- Summary of Aggregation Models
  - some cure underfitting; some cure overfitting**

- ③ Distilling Implicit Features: Extraction Models
  - next: extract features other than hypotheses**