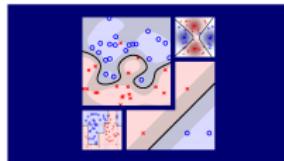


Machine Learning Techniques (機器學習技法)



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

- ① request size- N' data $\tilde{\mathcal{D}}_t$ by bootstrapping with \mathcal{D}
- ② obtain tree g_t by Randomized-DTree($\tilde{\mathcal{D}}_t$)

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

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

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

- ① reweight data by $\mathbf{u}^{(t)}$

每一層的資料會有一個weight: u_t

- ② obtain tree g_t by DTree($\mathcal{D}, \mathbf{u}^{(t)}$)
- ③ calculate ‘vote’ α_t of g_t

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

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

簡單來說，每一筆資料會有不同的權重、進而得到不同的小g

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}

根據權重來抽資料！

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

Weak Decision Tree Algorithm

α_t 就是每個小g最後的票數

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

if fully grown tree trained on all x_n

$\Rightarrow E_{in}(g_t) = 0$ if all x_n different

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

$\Rightarrow \epsilon_t = 0$

$\Rightarrow \alpha_t = \infty$ (**autocracy!!**) 因為給了一個小g無限大的票、等於只需要一棵樹就好

need: **pruned** tree trained on **some** x_n to be **weak**

- **pruned**: usual pruning, or just **limiting tree height**

- **some**: **sampling** $\propto u^{(t)}$ 所以樹不可以切到底、至少要做一點點的修剪（至少做到限制高度）

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

AdaBoost with Extremely-Pruned Tree

what if DTree with **height** ≤ 1 (extremely pruned)?

如果只配一棵最弱的樹會發生什麼事？

DTree (C&RT) with **height** ≤ 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 ϵ_t can be anything, even $\geq \frac{1}{2}$. Then, α_t can be ≤ 0 .

Example Weights of AdaBoost

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

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

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

- 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

可以證明， u_t 的總和會越來越小

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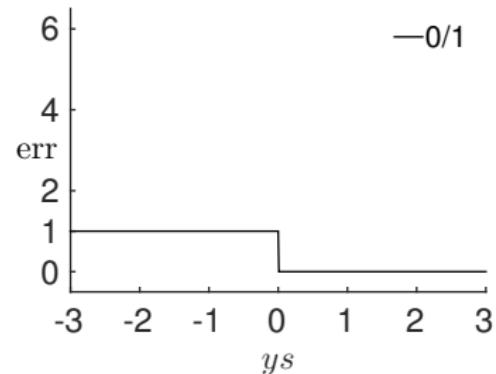
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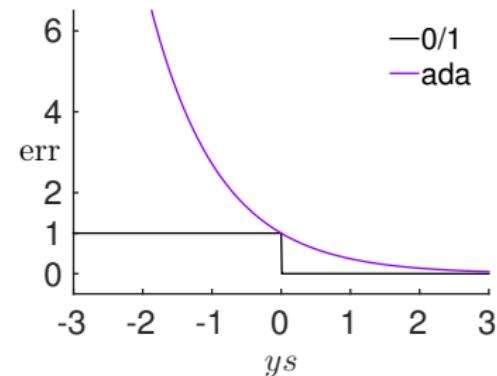
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$\widehat{\text{err}}_{\text{ADA}}$: **algorithmic error measure**
by **convex upper bound** of $\text{err}_{0/1}$

Gradient Descent on AdaBoost Error Function

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

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

梯度下降法：在某個點作泰勒展開後、看看往哪個方向會往下一點點，走完之後一直繼續下去

at iteration t , to find g_t , solve

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

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 η_t somewhat '**greedily faster**' than fixed (small) η
—called **steepest descent** for optimization 選擇某個方向後、在那個方向走最深！
- 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 η_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 η_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 η 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 η 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 $g_t = h$,

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

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

每個項乘上一個負號不影響平方

— 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 η 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 η 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

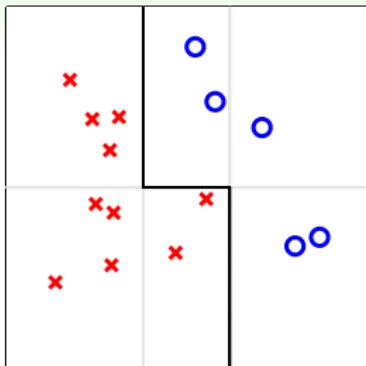
GradientBoost

GBDT

GradientBoost
+ 'weak' DTree

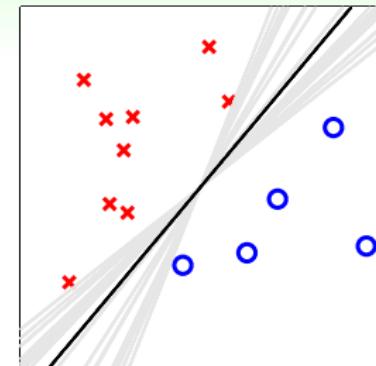
all three frequently used in practice

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**