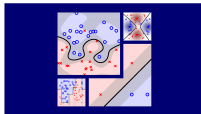


Machine Learning Techniques (機器學習技法)



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 $\mathbf{u}^{(t)}$
- 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($\mathcal{D}, \mathbf{u}^{(t)}$)

Weighted Decision Tree Algorithm

Weighted Algorithm

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

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 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** $\alpha_t = \ln \blacklozenge_t = \ln \sqrt{\frac{1-\epsilon_t}{\epsilon_t}}$ with **weighted error rate** ϵ_t

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

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

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

$\Rightarrow \epsilon_t = 0$

$\Rightarrow \alpha_t = \infty$ (**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** ≤ 1 (extremely pruned)?

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

$$\begin{aligned}
 u_n^{(t+1)} &= \begin{cases} u_n^{(t)} \cdot \blacklozenge_t & \text{if incorrect} \\ u_n^{(t)} / \blacklozenge_t & \text{if correct} \end{cases} \\
 &= u_n^{(t)} \cdot \blacklozenge_t^{-y_n g_t(\mathbf{x}_n)} = u_n^{(t)} \cdot \exp(-y_n \alpha_t g_t(\mathbf{x}_n))
 \end{aligned}$$

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

- 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}

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

Voting Score and Margin

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

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

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

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

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

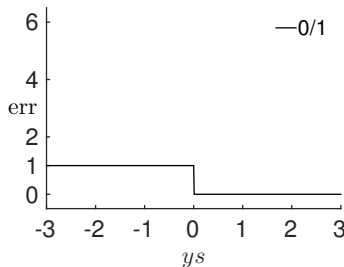
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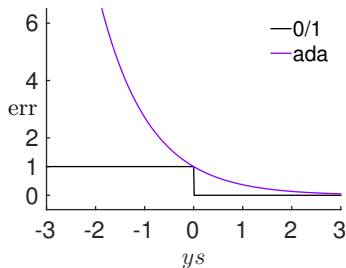
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- $\text{err}_{0/1}(s, y) = \mathbb{I}[ys \leq 0]$
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$\widehat{\text{err}}_{\text{ADA}}$: **algorithmic error measure**
by **convex upper bound** of $\text{err}_{0/1}$

Gradient Descent on AdaBoost Error Function

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

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

at iteration t , to find g_t , solve

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

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 $\in \{-1, +1\}$:

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

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

\mathcal{A} : good $g_t = h$ for ‘gradient descent’

Deciding Blending Weight as Optimization

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

after finding g_t , how about $\min_{\eta} \hat{E}_{\text{ADA}} = \sum_{n=1}^N u_n^{(t)} \exp(-y_n \eta g_t(\mathbf{x}_n))$

- optimal η_t somewhat ‘**greedily faster**’ than fixed (small) η —called **steepest** descent for optimization
- 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)
- $\hat{E}_{\text{ADA}} = \left(\sum_{n=1}^N u_n^{(t)} \right) \cdot \left((1 - \epsilon_t) \exp(-\eta) + \epsilon_t \exp(+\eta) \right)$

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

Fun Time

With $\hat{E}_{\text{ADA}} = \left(\sum_{n=1}^N u_n^{(t)} \right) \cdot \left((1 - \epsilon_t) \exp(-\eta) + \epsilon_t \exp(+\eta) \right)$, which of the following is $\frac{\partial \hat{E}_{\text{ADA}}}{\partial \eta}$ 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 $\hat{E}_{\text{ADA}} = \left(\sum_{n=1}^N u_n^{(t)} \right) \cdot \left((1 - \epsilon_t) \exp(-\eta) + \epsilon_t \exp(+\eta) \right)$, which of the following is $\frac{\partial \hat{E}_{\text{ADA}}}{\partial \eta}$ 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

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

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

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

Learning Hypothesis as Optimization

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

- **magnitude** of h does not matter: because η will be optimized next
- **penalize large magnitude** to avoid naïve solution

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

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

GradientBoost for regression:

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

Deciding Blending Weight as Optimization

after finding $g_t = h$,

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

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

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

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

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 $\mathcal{A}(\{(\mathbf{x}_n, y_n - s_n)\})$ where \mathcal{A} is a (squared-error) regression algorithm

—**how about sampled and pruned C&RT?**

- 2 compute $\alpha_t = \text{OneVarLinearRegression}(\{(g_t(\mathbf{x}_n), y_n - s_n)\})$

- 3 update $s_n \leftarrow s_n + \alpha_t g_t(\mathbf{x}_n)$

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

AdaBoost

Decision Tree

Random Forest

randomized bagging
+ 'strong' DTree

AdaBoost-DTree

AdaBoost
+ 'weak' DTree

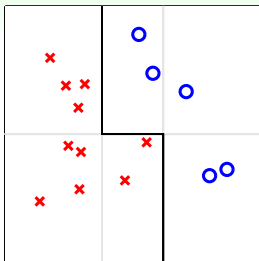
GradientBoost

GBDT

GradientBoost
+ 'weak' DTree

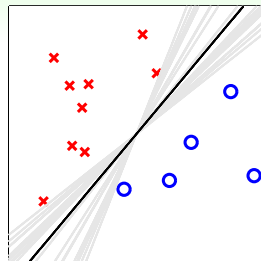
all three frequently used in practice

Specialty of Aggregation Models



cure underfitting

- $G(\mathbf{x})$ 'strong'
- aggregation
 \Rightarrow **feature transform**



cure overfitting

- $G(\mathbf{x})$ 'moderate'
- aggregation
 \Rightarrow **regularization**

proper aggregation (a.k.a. 'ensemble')
 \Rightarrow **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**