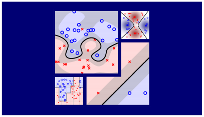
Machine Learning Techniques
(機器學習技法)



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

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

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 $\mathbf{x}_n$

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

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

$\Longrightarrow \epsilon_t = 0$

$\Longrightarrow \alpha_t = \infty$ (**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 $\tilde{\mathcal{D}}_t$, 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

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

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

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

- 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: $u_n^{(T+1)} \propto \exp(-y_n($ 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** = $\frac{y_n \cdot (\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n) + b)}{\|\mathbf{w}\|}$, **remember? :-)**

y_n(voting score) = signed & unnormalized **margin**

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

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

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

AdaBoost Error Function

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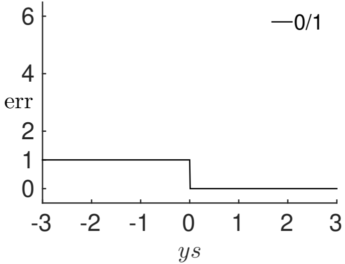

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AdaBoost Error Function

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

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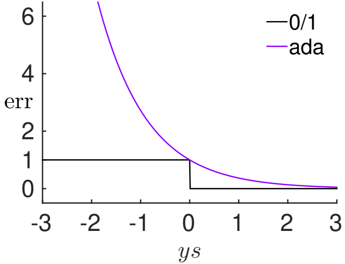


$\widehat{\mathrm{err}}_{\mathrm{ADA}}$: **algorithmic error measure** by **convex upper bound** of $\mathrm{err}_{0/1}$

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

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

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

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

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

- 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)
- $\widehat{E}_{\text{ADA}} = \left(\sum_{n=1}^{N} u_n^{(t)}\right) \cdot \left((1-\epsilon_t)\exp(-\eta) + \epsilon_t \exp(+\eta)\right)$

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

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

with any hypothesis h (usually real-output hypothesis)

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

GradientBoost for Regression

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

$$\min_{h} \ldots \overset{\text{taylor}}{\approx} \min_{h} \quad \frac{1}{N}\sum_{n=1}^{N} \underbrace{\text{err}\left(s_n, y_n\right)}_{\text{constant}} + \frac{1}{N}\sum_{n=1}^{N} \eta h(\mathbf{x}_n) \left.\frac{\partial \text{err}(s, y_n)}{\partial s}\right|_{s=s_n}$$

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

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

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

- 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 $g_t = h$,

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

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

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

GradientBoost for regression: $\alpha_t =$ optimal η
by g_t-transformed linear regression

Putting Everything Together

Gradient Boosted Decision Tree (GBDT)

$s_1 = s_2 = \ldots = s_N = 0$

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

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

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

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

Fun Time

Which of the following is the optimal η for

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

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

Reference Answer: 2

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

Map of Blending Models

blending: aggregate after getting **diverse** g_t

uniform	non-uniform	conditional
simple voting/averaging of g_t	linear model on g_t-transformed inputs	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

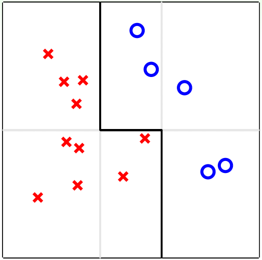
AdaBoost-DTree
AdaBoost
+ 'weak' DTree

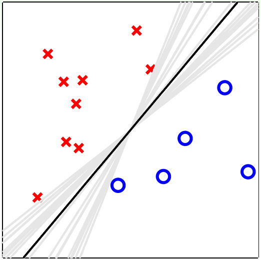
GradientBoost

GBDT
GradientBoost
+ 'weak' DTree

all three frequently used in practice

Specialty of Aggregation Models





cure underfitting

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

cure overfitting

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

proper aggregation (a.k.a. 'ensemble')
$\Longrightarrow$ **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 grad. 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**