Machine Learning Techniques

(機器學習技法)



Lecture 11: Gradient Boosted Decision Tree

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Roadmap

- 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

```
function RandomForest(\mathcal{D})
```

For t = 1, 2, ..., 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 $G = Uniform(\{g_t\})$

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function AdaBoost-DTree(D) For t = 1, 2, ..., T

 $\mathbf{0}$ reweight data by $\mathbf{u}^{(t)}$

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

Weighted Algorithm

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

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

'Weighted' Algorithm in Bagging

weights **u** expressed by bootstrap-sampled copies

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

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DTree (C&RT) with **height** ≤ 1

learn branching criteria

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

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-if impurity = binary classification error,

just a decision stump, remember? :-)

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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?

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

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- $\alpha_t = 0$
- $\alpha_t > 0$
- 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

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

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ee Optimization View of AdaBoost Example Weights of AdaBoost

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

linear blending = LinModel + hypotheses as transform + constraints

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want y_n (voting score) **positive & large** exp($-y_n$ (voting score)) **small**

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

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

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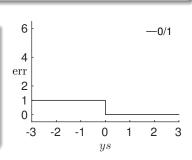
linear score
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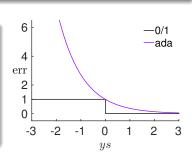


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- $\operatorname{err}_{0/1}(s, y) = [ys \le 0]$
- err_{ADA}(s, y) = exp(-ys):
 upper bound of err_{0/1}
 —called exponential error measure

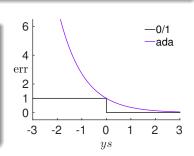


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- err_{ADA}(s, y) = exp(-ys):
 upper bound of err_{0/1}
 —called exponential error
 measure



err_{ADA}: algorithmic error measure by convex upper bound of err_{0/1}

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

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

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

recall: gradient descent (remember?:-)), at iteration
$$t$$
 min $E_{\text{in}}(\mathbf{w}_t + \eta \mathbf{v}) \approx \underbrace{E_{\text{in}}(\mathbf{w}_t)}_{\text{known}} + \underbrace{\eta}_{\text{given positive}} \underbrace{\nabla E_{\text{in}}(\mathbf{w}_t)}_{\text{known}}$

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= \sum_{n=1}^{N} \exp \left(-y_n \eta h(\mathbf{x}_n) \right)$$

recall: gradient descent (remember?:-)), at iteration
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$$= \sum_{n=1}^{N} u_n^{(t)} \exp\left(-y_n \eta h(\mathbf{x}_n)\right)$$

recall: gradient descent (remember?:-)), at iteration
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$$\stackrel{\text{taylor}}{\approx} \sum_{n=1}^{N} u_n^{(t)} ()$$

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

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$$= \sum_{n=1}^{N} u_n^{(t)} \exp\left(-y_n \frac{\eta}{\eta} h(\mathbf{x}_n)\right)$$

$$\stackrel{\text{taylor}}{\approx} \sum_{n=1}^{N} u_n^{(t)} \left(1 - y_n \frac{\eta}{\eta} h(\mathbf{x}_n)\right)$$

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

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

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

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

$$\stackrel{\text{taylor}}{\approx} \sum_{n=1}^{N} u_n^{(t)} \left(1 - y_n \eta h(\mathbf{x}_n)\right) = \sum_{n=1}^{N} u_n^{(t)} - \eta \sum_{n=1}^{N} u_n^{(t)}$$

recall: gradient descent (remember?:-)), at iteration
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$$\min_{\|\mathbf{v}\|=1} E_{\text{in}}(\mathbf{w}_t + \eta \mathbf{v}) \approx \underbrace{E_{\text{in}}(\mathbf{w}_t)}_{\text{known}} + \underbrace{\eta}_{\text{given positive}} \mathbf{v}^T \underbrace{\nabla E_{\text{in}}(\mathbf{w}_t)}_{\text{known}}$$

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\stackrel{\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)$$

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

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

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

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

$$\sum_{n=1}^{N} u_n^{(t)} \left(-y_n h(\mathbf{x}_n) \right) = \sum_{n=1}^{N} u_n^{(t)} \left\{ \begin{array}{cc} -1 & \text{if } y_n = h(\mathbf{x}_n) \\ +1 & \text{if } y_n \neq h(\mathbf{x}_n) \end{array} \right.$$

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

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$$= -\sum_{n=1}^{N} u_n^{(t)} + 2 \qquad \cdot N$$

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

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$$= -\sum_{n=1}^{N} u_n^{(t)} + 2E_{\text{in}}^{\mathbf{u}^{(t)}}(h) \cdot N$$

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

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—who minimizes $E_{in}^{\mathbf{u}^{(t)}}(h)$?

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

A: **good** $g_t = h$ for 'gradient descent'

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

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• optimal η_t somewhat 'greedily faster' than fixed (small) η

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- two cases inside summation:
 - $y_n = g_t(\mathbf{x}_n)$:

(correct)

• $y_n \neq g_t(\mathbf{x}_n)$:

AdaBoost finds
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- 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)

• $V_n \neq g_t(\mathbf{x}_n)$: $u_n^{(t)} \exp(+\eta)$

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

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(correct)

• $\mathbf{v}_n \neq \mathbf{g}_t(\mathbf{x}_n)$: $u_n^{(t)} \exp(+\eta)$

•
$$\widehat{E}_{ADA} = \left(\sum_{n=1}^{N} u_n^{(t)}\right) \cdot \left($$

$$\exp\left(-\frac{\eta}{\eta}\right) + \exp\left(+\frac{\eta}{\eta}\right)$$

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: $u_n^{(t)} \exp(+\eta)$

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

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two cases inside summation:

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$$y_n = g_t(\mathbf{x}_n) : u_n^{(t)} \exp(-\eta)$$

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

by solving
$$\frac{\partial \widehat{\mathcal{E}}_{ADA}}{\partial_{\pmb{\eta}}}=0$$
, steepest $\eta_t=\ln\sqrt{\frac{1-\epsilon_t}{\epsilon_t}}=$

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

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

by solving
$$\frac{\partial \widehat{E}_{\text{ADA}}}{\partial \eta}=0$$
, steepest $\eta_t=\ln\sqrt{\frac{1-\epsilon_t}{\epsilon_t}}=lpha_t$, remember? :-)

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

- 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)

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

by solving $\frac{\partial \widehat{E}_{ADA}}{\partial \eta} = 0$, steepest $\eta_t = \ln \sqrt{\frac{1 - \epsilon_t}{\epsilon_t}} = \alpha_t$, remember? :-)

—AdaBoost: steepest descent with approximate functional gradient

Fun Time

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

Fun Time

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

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

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

with binary-output hypothesis h

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

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

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

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

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

with any hypothesis h (usually real-output hypothesis)

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

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

with any hypothesis h (usually real-output hypothesis)

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

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

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

$$\underset{h}{\min} \dots \underset{h}{\approx} \underset{n=1}{\min} \quad \frac{1}{N} \sum_{n=1}^{N} \underbrace{\operatorname{err}(s_{n}, y_{n})}_{\text{constant}} + \frac{1}{N} \sum_{n=1}^{N} \eta h(\mathbf{x}_{n})$$

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

$$\underset{h}{\text{min} \dots} \approx \underset{h}{\text{min}} \frac{1}{N} \sum_{n=1}^{N} \underbrace{\operatorname{err}(s_n, y_n)}_{\text{constant}} + \frac{1}{N} \sum_{n=1}^{N} \frac{\eta h(\mathbf{x}_n)}{\partial s} \left| \frac{\partial \operatorname{err}(s, y_n)}{\partial s} \right|_{s=s_n}$$

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

$$\frac{\min_{h} \dots}{\approx} \frac{1}{N} \sum_{n=1}^{N} \underbrace{\operatorname{err}(s_{n}, y_{n})}_{\text{constant}} + \frac{1}{N} \sum_{n=1}^{N} \frac{\eta}{\eta} h(\mathbf{x}_{n}) \frac{\partial \operatorname{err}(s, y_{n})}{\partial s} \Big|_{s=s_{n}}$$

$$= \min_{h} \operatorname{constants} + \frac{\eta}{N} \sum_{n=1}^{N} h(\mathbf{x}_{n}) \cdot \frac{\partial \operatorname{err}(s, y_{n})}{\partial s} \Big|_{s=s_{n}}$$

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

$$\frac{\min_{h} \dots}{\approx} \frac{1}{N} \sum_{n=1}^{N} \underbrace{\operatorname{err}(s_{n}, y_{n})}_{\text{constant}} + \frac{1}{N} \sum_{n=1}^{N} \frac{\eta h(\mathbf{x}_{n})}{\partial s} \frac{\partial \operatorname{err}(s, y_{n})}{\partial s} \Big|_{s=s_{n}}$$

$$= \min_{h} \operatorname{constants} + \frac{\eta}{N} \sum_{n=1}^{N} h(\mathbf{x}_{n}) \cdot 2(s_{n} - y_{n})$$

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

$$\frac{\min \dots}{h} \stackrel{\text{taylor}}{\approx} \min_{h} \frac{1}{N} \sum_{n=1}^{N} \underbrace{\text{err}(s_{n}, y_{n})}_{\text{constant}} + \frac{1}{N} \sum_{n=1}^{N} \eta h(\mathbf{x}_{n}) \frac{\partial \text{err}(s, y_{n})}{\partial s} \Big|_{s=s_{n}}$$

$$= \min_{h} \text{constants} + \frac{\eta}{N} \sum_{n=1}^{N} h(\mathbf{x}_{n}) \cdot 2(s_{n} - y_{n})$$

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

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

$$\frac{\min \dots}{h} \stackrel{\text{taylor}}{\approx} \min_{h} \frac{1}{N} \sum_{n=1}^{N} \underbrace{\text{err}(s_{n}, y_{n})}_{\text{constant}} + \frac{1}{N} \sum_{n=1}^{N} \eta h(\mathbf{x}_{n}) \frac{\partial \text{err}(s, y_{n})}{\partial s} \Big|_{s=s_{n}}$$

$$= \min_{h} \text{constants} + \frac{\eta}{N} \sum_{n=1}^{N} h(\mathbf{x}_{n}) \cdot 2(s_{n} - y_{n})$$

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

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

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

magnitude of h does not matter:

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

• magnitude of h does not matter: because η will be optimized next

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

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

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

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

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

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

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

$$\min_{h} \quad \text{constants} + \frac{\eta}{N} \sum_{n=1}^{N} \left(2h(\mathbf{x}_{n})(s_{n} - y_{n}) + (h(\mathbf{x}_{n}))^{2} \right)$$

$$= \quad \text{constants} + \frac{\eta}{N} \sum_{n=1}^{N} \left(\frac{1}{N} \left(\frac{1}{N} \right) \left(\frac{$$

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

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

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

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

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

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

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

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

• solution of penalized approximate functional gradient: squared-error regression on $\{(\mathbf{x}_n, \underline{y}_n - \underline{s}_n)\}$

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

- magnitude of h does not matter: because η will be optimized next
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$$\min_{h} \quad \text{constants} + \frac{\eta}{N} \sum_{n=1}^{N} \left(2h(\mathbf{x}_n)(s_n - y_n) + (h(\mathbf{x}_n))^2 \right)$$

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

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

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

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

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

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

• solution of penalized approximate functional gradient: squared-error regression on $\{(\mathbf{x}_n, \underline{y}_n - \underline{s}_n)\}$

GradientBoost for regression:

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

$$\min_{\eta} \min_{n \to \infty} \frac{1}{N} \sum_{n=1}^{N} \operatorname{err} \left(\sum_{\tau=1}^{t-1} \alpha_{\tau} g_{\tau}(\mathbf{x}_{n}) + \eta g_{t}(\mathbf{x}_{n}), y_{n} \right) \text{ with } \operatorname{err}(s, y) = (s - y)^{2}$$

$$\min_{\eta} \min_{N} \sum_{n=1}^{N} \operatorname{err} \left(\sum_{\tau=1}^{t-1} \alpha_{\tau} g_{\tau}(\mathbf{x}_{n}) + \eta g_{t}(\mathbf{x}_{n}), y_{n} \right) \text{ with } \operatorname{err}(s, y) = (s - y)^{2}$$

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

$$\min_{\eta} \min_{N} \sum_{n=1}^{N} \operatorname{err} \left(\sum_{\tau=1}^{t-1} \alpha_{\tau} g_{\tau}(\mathbf{x}_{n}) + \eta g_{t}(\mathbf{x}_{n}), y_{n} \right) \text{ with } \operatorname{err}(s, y) = (s - y)^{2}$$

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

$$\min_{\eta} \min_{N} \sum_{n=1}^{N} \operatorname{err} \left(\sum_{\tau=1}^{t-1} \alpha_{\tau} g_{\tau}(\mathbf{x}_{n}) + \eta g_{t}(\mathbf{x}_{n}), y_{n} \right) \text{ with } \operatorname{err}(s, y) = (s - y)^{2}$$

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

after finding $g_t = h$,

$$\min_{\eta} \min_{n \to \infty} \frac{1}{N} \sum_{n=1}^{N} \operatorname{err} \left(\sum_{\tau=1}^{t-1} \alpha_{\tau} g_{\tau}(\mathbf{x}_{n}) + \eta g_{t}(\mathbf{x}_{n}), y_{n} \right) \text{ with } \operatorname{err}(s, y) = (s - y)^{2}$$

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

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

after finding $g_t = h$,

$$\min_{\eta} \min_{N} \sum_{n=1}^{N} \operatorname{err} \left(\sum_{\tau=1}^{t-1} \alpha_{\tau} g_{\tau}(\mathbf{x}_{n}) + \eta g_{t}(\mathbf{x}_{n}), y_{n} \right) \text{ with } \operatorname{err}(s, y) = (s - y)^{2}$$

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

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

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

Gradient Boosted Decision Tree (GBDT)

for
$$t = 1, 2, ..., T$$

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

Gradient Boosted Decision Tree (GBDT)

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

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

1 obtain g_t by $\mathcal{A}(\{(\mathbf{x}_n, \mathbf{y}_n - \mathbf{s}_n)\})$ where \mathcal{A} is a (squared-error) regression algorithm

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

Gradient Boosted Decision Tree (GBDT)

$$s_1 = s_2 = \ldots = s_N = 0$$
 for $t = 1, 2, \ldots, T$

1 obtain g_t by $\mathcal{A}(\{(\mathbf{x}_n, \mathbf{y}_n - \mathbf{s}_n)\})$ where \mathcal{A} is a (squared-error) regression algorithm

—how about sampled and pruned C&RT?

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

Gradient Boosted Decision Tree (GBDT)

```
s_1 = s_2 = \ldots = s_N = 0 for t = 1, 2, \ldots, T
```

- 1 obtain g_t by $\mathcal{A}(\{(\mathbf{x}_n, \mathbf{y}_n \mathbf{s}_n)\})$ where \mathcal{A} is a (squared-error) regression algorithm
- —how about sampled and pruned C&RT?
- 2 compute α_t = OneVarLinearRegression({ $\{(g_t(\mathbf{x}_n), y_n s_n)\}$ })

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

Gradient Boosted Decision Tree (GBDT)

```
s_1 = s_2 = \ldots = s_N = 0
for t = 1, 2, \ldots, T
```

- obtain g_t by $\mathcal{A}(\{(\mathbf{x}_n, \mathbf{y}_n \mathbf{s}_n)\})$ where \mathcal{A} is a (squared-error) regression algorithm
 - —how about sampled and pruned C&RT?
- 2 compute α_t = 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 $G(\mathbf{x}) = \sum_{t=1}^{T} \alpha_t g_t(\mathbf{x})$

Gradient Boosted Decision Tree (GBDT)

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

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

- 1 obtain g_t by $\mathcal{A}(\{(\mathbf{x}_n, \mathbf{y}_n \mathbf{s}_n)\})$ where \mathcal{A} is a (squared-error) regression algorithm
- —how about sampled and pruned C&RT?
- 2 compute α_t = 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 $(\sum_{n=1}^{N} q_t(\mathbf{x}_n)(y_n s_n)) (\sum_{n=1}^{N} q_t^2(\mathbf{x}_n))$

Fun Time

Which of the following is the optimal η for

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

- 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** $(\sum_{n=1}^{N} q_t(\mathbf{x}_n)(y_n s_n)) (\sum_{n=1}^{N} q_t^2(\mathbf{x}_n))$

Reference Answer: (2)

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

blending: aggregate after getting diverse g_t

blending: aggregate after getting diverse g_t

uniform

simple voting/averaging of g_t

blending: aggregate after getting diverse g_t

 $\begin{array}{c} \text{uniform} & \text{non-uniform} \\ \text{simple} & \text{linear model on} \\ \text{voting/averaging of } g_t & g_{t}\text{-transformed inputs} \end{array}$

blending: aggregate after getting diverse g_t

 $\begin{array}{c|cccc} \text{uniform} & \text{non-uniform} & \text{conditional} \\ \text{simple} & \text{linear model on} & \text{nonlinear model on} \\ \text{voting/averaging of } g_t & g_t\text{-transformed inputs} & g_t\text{-transformed inputs} \\ \end{array}$

blending: aggregate after getting diverse g_t

 $\begin{array}{c|cccc} \text{uniform} & \text{non-uniform} & \text{conditional} \\ \text{simple} & \text{linear model on} \\ \text{voting/averaging of } g_t & g_{t}\text{-transformed inputs} & g_{t}\text{-transformed inputs} \\ \end{array}$

uniform for 'stability';

blending: aggregate after getting diverse g_t

$\begin{array}{c|cccc} \text{uniform} & \text{non-uniform} & \text{conditional} \\ \text{simple} & \text{linear model on} \\ \text{voting/averaging of } g_t & g_t\text{-transformed inputs} & g_t\text{-transformed inputs} \end{array}$

uniform for 'stability'; non-uniform/conditional carefully for 'complexity'

learning: aggregate as well as getting diverse g_t

learning: aggregate as well as getting diverse g_t

Bagging

diverse g_t by bootstrapping;

learning: aggregate as well as getting diverse g_t

Bagging

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

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;

learning: aggregate as well as getting diverse g_t

BaggingAdaBoostdiverse g_t by
bootstrapping;
uniform vote
by nothing :-)diverse g_t
by reweighting;
linear vote
by steepest search

learning: aggregate as well as getting diverse gt

Bagging	AdaBoost	Decision Tree
diverse g_t by	diverse g _t	
bootstrapping;	by reweighting;	
uniform vote	linear vote	conditional vote
by nothing :-)	by steepest search	by branching

learning: aggregate as well as getting diverse g_t

BaggingAdaBoostDecision Treediverse g_t by
bootstrapping;
uniform vote
by nothing:-)diverse g_t diverse g_t
by reweighting;
linear vote
by steepest searchby data splitting;
conditional vote
by branching

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;

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

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

Bagging AdaBoost Decision Tree

GradientBoost

Bagging

AdaBoost

Decision Tree

Random Forest

randomized bagging + 'strong' DTree

GradientBoost

Random Forest
randomized bagging
+ 'strong' DTree

GradientBoost

AdaBoost

AdaBoost
- 'weak' DTree

GradientBoost

Bagging AdaBoost Random Forest AdaBoost-DTree randomized bagging AdaBoost + 'strong' DTree + 'weak' DTree GradientBoost **GBDT** GradientBoost + 'weak' DTree

Decision Tree

Bagging AdaBoost Random Forest randomized bagging + 'strong' DTree

AdaBoost-DTree

AdaBoost

+ 'weak' DTree

GradientBoost

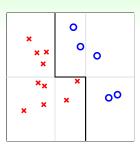
GBDT

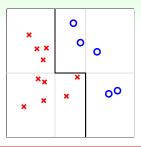
GradientBoost

+ 'weak' DTree

all three frequently used in practice

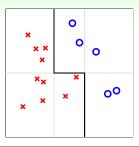
Decision Tree





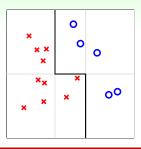
cure underfitting

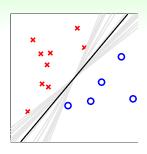
• $G(\mathbf{x})$ 'strong'



cure underfitting

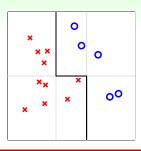
- G(x) 'strong'
- aggregation
 - **⇒** feature transform

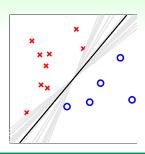




cure underfitting

- G(x) 'strong'
- aggregation
 - ⇒ feature transform



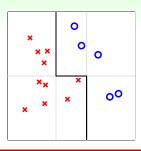


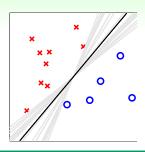
cure underfitting

- G(x) 'strong'
- aggregation
 - **⇒** feature transform

cure overfitting

G(x) 'moderate'



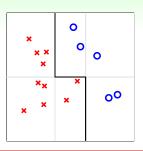


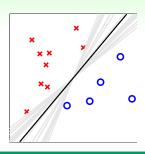
cure underfitting

- G(x) 'strong'
- aggregation
 - **⇒** feature transform

cure overfitting

- G(x) 'moderate'
- aggregation
 - ⇒ regularization





cure underfitting

- *G*(**x**) 'strong'
- aggregation
 - ⇒ feature transform

cure overfitting

- G(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?

- 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?

- AdaBoost
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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