Machine Learning
(機器學習)

Lecture 13: Decision Tree Ensembles

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Roadmap

1. When Can Machines Learn?
2. Why Can Machines Learn?
3. How Can Machines Learn?
4. How Can Machines Learn Better?
5. Embedding Numerous Features: Kernel Models
6. Combining Predictive Features: Aggregation Models

Lecture 13: Decision Tree Ensembles

- Decision Tree Hypothesis
- Decision Tree Algorithm
- Decision Tree in Action
- Random Forest Algorithm
- Out-Of-Bag Estimate
- Random Forest in Action
- Optimization View of AdaBoost
- Gradient Boosting
- Summary of Aggregation Models

What We Have Done

blending: aggregate after getting g_t;
learning: aggregate as well as getting g_t

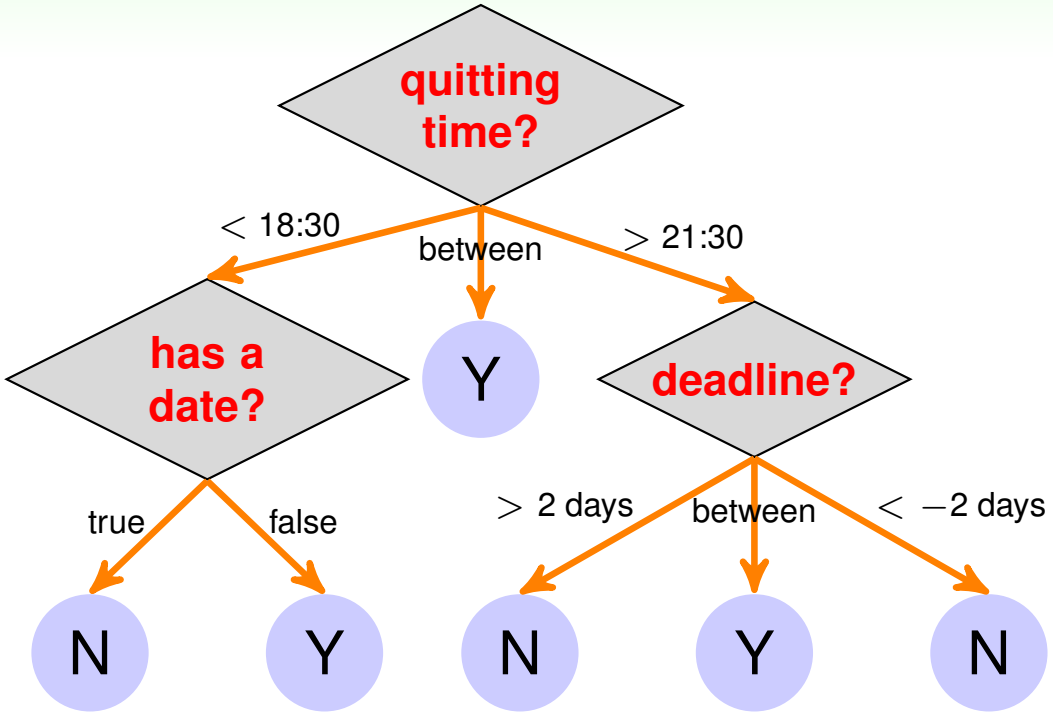
aggregation type	blending	learning
uniform	voting/averaging	Bagging
non-uniform	linear	AdaBoost
conditional	stacking	**Decision Tree**

decision tree: a traditional learning model that realizes **conditional aggregation**

Decision Tree for Watching MOOC Lectures

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

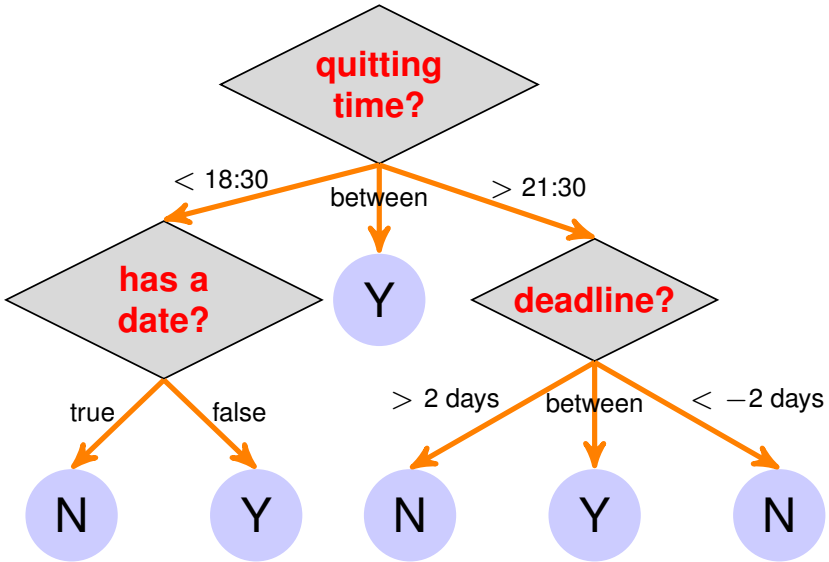
- **base hypothesis** $g_t(\mathbf{x})$: leaf at end of path t, a **constant** here
- **condition** $q_t(\mathbf{x})$: ⟦is $\mathbf{x}$ on path t?⟧
- usually with **simple internal nodes**



decision tree: arguably one of the most **human-mimicking models**

Recursive View of Decision Tree

Path View: $G(\mathbf{x}) = \sum_{t=1}^{T} [\![\mathbf{x} \text{ on path } t]\!] \cdot \text{leaf}_t(\mathbf{x})$



Recursive View

$$G(\mathbf{x}) = \sum_{c=1}^{C} [\![b(\mathbf{x}) = c]\!] \cdot G_c(\mathbf{x})$$

- $G(\mathbf{x})$: full-tree hypothesis
- $b(\mathbf{x})$: branching criteria
- $G_c(\mathbf{x})$: sub-tree hypothesis at the c-th branch

tree = (root, sub-trees), just like what **your data structure instructor would say :-)**

Disclaimers about Decision Tree

Usefulness

- human-explainable: **widely used** in business/medical data analysis
- simple: **even freshmen can implement one :-)**
- efficient in prediction and **training**

However.....

- heuristic: mostly **little theoretical** explanations
- heuristic**s**: 'heuristic**s** selection' confusing to beginners
- arguably no single **representative algorithm**

decision tree: mostly **heuristic** **but useful** on its own

Questions?

A Basic Decision Tree Algorithm

$$G(\mathbf{x}) = \sum_{c=1}^{C} [\![b(\mathbf{x}) = c]\!] \, G_c(\mathbf{x})$$

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, y_n)\}_{n=1}^{N}$)

if termination criteria met

return base hypothesis $g_t(\mathbf{x})$

else

1. learn branching criteria $b(\mathbf{x})$
2. split $\mathcal{D}$ to C parts $\mathcal{D}_c = \{(\mathbf{x}_n, y_n) : b(\mathbf{x}_n) = c\}$
3. build sub-tree $G_c \leftarrow$ DecisionTree($\mathcal{D}_c$)
4. return $G(\mathbf{x}) = \sum_{c=1}^{C} [\![b(\mathbf{x}) = c]\!] \, G_c(\mathbf{x})$

four choices: number of branches, branching criteria, termination criteria, & base hypothesis

Classification and Regression Tree (C&RT)

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, y_n)\}_{n=1}^{N}$)
if termination criteria met
    return base hypothesis $g_t(\mathbf{x})$
else ...
    2 split $\mathcal{D}$ to C parts $\mathcal{D}_c = \{(\mathbf{x}_n, y_n) : b(\mathbf{x}_n) = c\}$

two simple choices

- $C = 2$ (binary tree)
- $g_t(\mathbf{x}) = E_{\text{in}}$-optimal constant
  - binary/multiclass classification (0/1 error): majority of $\{y_n\}$
  - regression (squared error): average of $\{y_n\}$

disclaimer:
C&RT here is based on **selected components** of **CART^{TM} of California Statistical Software**

Branching in C&RT: Purifying

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, y_n)\}_{n=1}^{N}$)
if termination criteria met
    return base hypothesis $g_t(\mathbf{x})$ = E_{in}-optimal constant
else ...
1. learn branching criteria $b(\mathbf{x})$
2. split $\mathcal{D}$ to 2 parts $\mathcal{D}_c = \{(\mathbf{x}_n, y_n) : b(\mathbf{x}_n) = c\}$

more simple choices

- simple internal node for $C = 2$: $\{1, 2\}$**-output decision stump**
- 'easier' sub-tree: branch by **purifying**

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

C&RT: **bi-branching** by **purifying**

Impurity Functions

by E_{in} of optimal constant

- regression error:

$$\text{impurity}(\mathcal{D}) = \frac{1}{N}\sum_{n=1}^{N}(y_n - \bar{y})^2$$

with $\bar{y}$ = average of $\{y_n\}$

- classification error:

$$\text{impurity}(\mathcal{D}) = \frac{1}{N}\sum_{n=1}^{N}[\![y_n \neq y^*]\!]$$

with y^* = majority of $\{y_n\}$

for classification

- Gini index:

$$1 - \sum_{k=1}^{K}\left(\frac{\sum_{n=1}^{N}[\![y_n = k]\!]}{N}\right)^2$$

—all k considered together

- classification error:

$$1 - \max_{1\le k\le K}\frac{\sum_{n=1}^{N}[\![y_n = k]\!]}{N}$$

—optimal $k = y^*$ only

popular choices: **Gini** for classification, **regression error** for regression

Termination in C&RT

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, y_n)\}_{n=1}^{N}$)
if termination criteria met
    return base hypothesis $g_t(\mathbf{x})$ = E_{in}-optimal constant
else ...
1. learn branching criteria

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

'forced' to terminate when

- all y_n the same: impurity = 0 $\Longrightarrow$ $g_t(\mathbf{x}) = y_n$
- all $\mathbf{x}_n$ the same: **no decision stumps**

C&RT: **fully-grown tree** with constant leaves
that come from **bi-branching** by **purifying**

Basic C&RT Algorithm

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, y_n)\}_{n=1}^{N}$)

if cannot branch anymore

return $g_t(\mathbf{x}) = E_{\text{in}}$-optimal constant

else

1. learn branching criteria

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

2. split $\mathcal{D}$ to 2 parts $\mathcal{D}_c = \{(\mathbf{x}_n, y_n) : b(\mathbf{x}_n) = c\}$
3. build sub-tree $G_c \leftarrow \text{DecisionTree}(\mathcal{D}_c)$
4. return $G(\mathbf{x}) = \sum_{c=1}^{2} [\![b(\mathbf{x}) = c]\!] \, G_c(\mathbf{x})$

easily handle binary classification, regression, & **multi-class classification**

Regularization by Pruning

fully-grown tree: $E_{\text{in}}(G) = 0$ if all $\mathbf{x}_n$ different
but **overfit** (large E_{out}) because **low-level trees built with small** $\mathcal{D}_c$

- need a **regularizer**, say, $\Omega(G) = \text{NumberOfLeaves}(G)$
- want **regularized** decision tree:

$$\underset{\text{all possible } G}{\text{argmin}} \quad E_{\text{in}}(G) + \lambda\Omega(G)$$

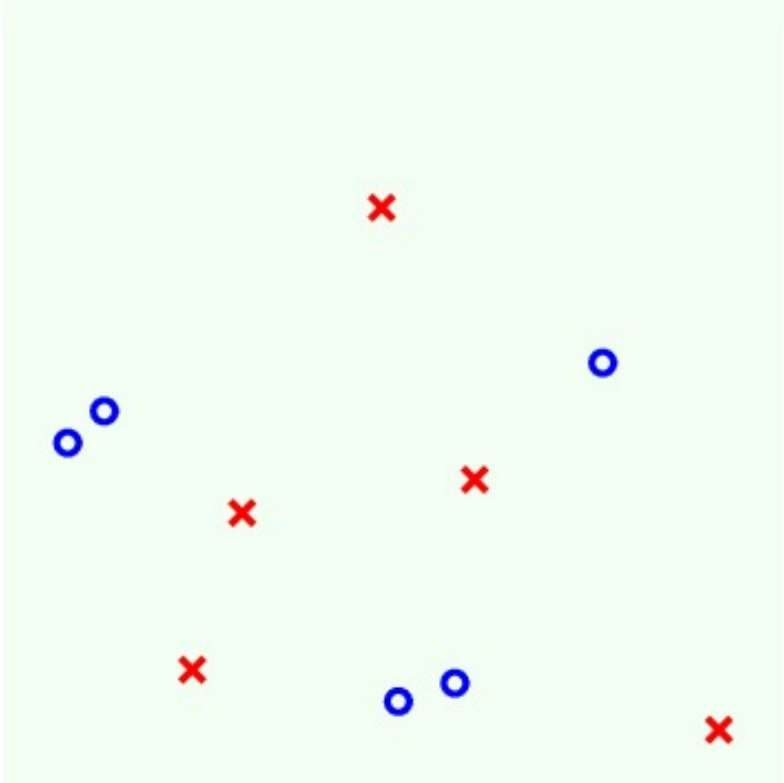
—called **pruned** decision tree

- heuristic mature & prevalent in many decision tree algorithms (details omitted)

systematic choice of λ? **validation**

Questions?

A Simple Data Set



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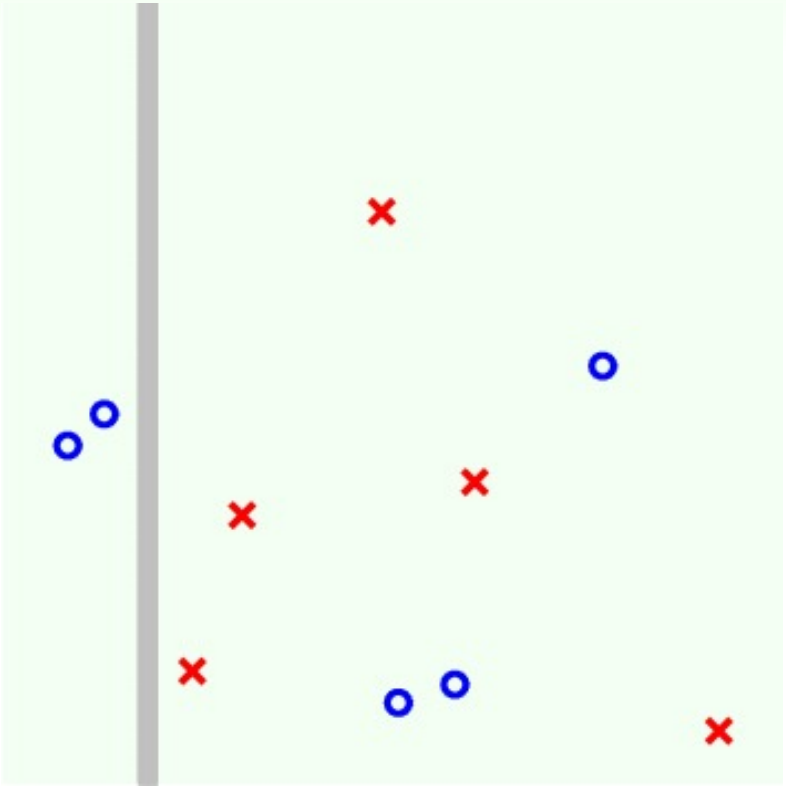

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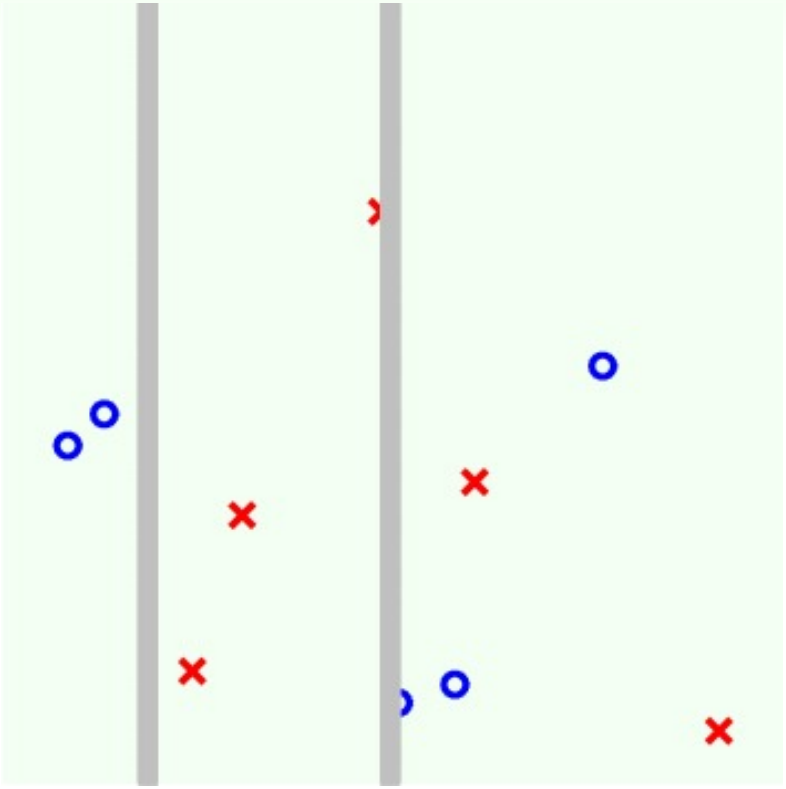

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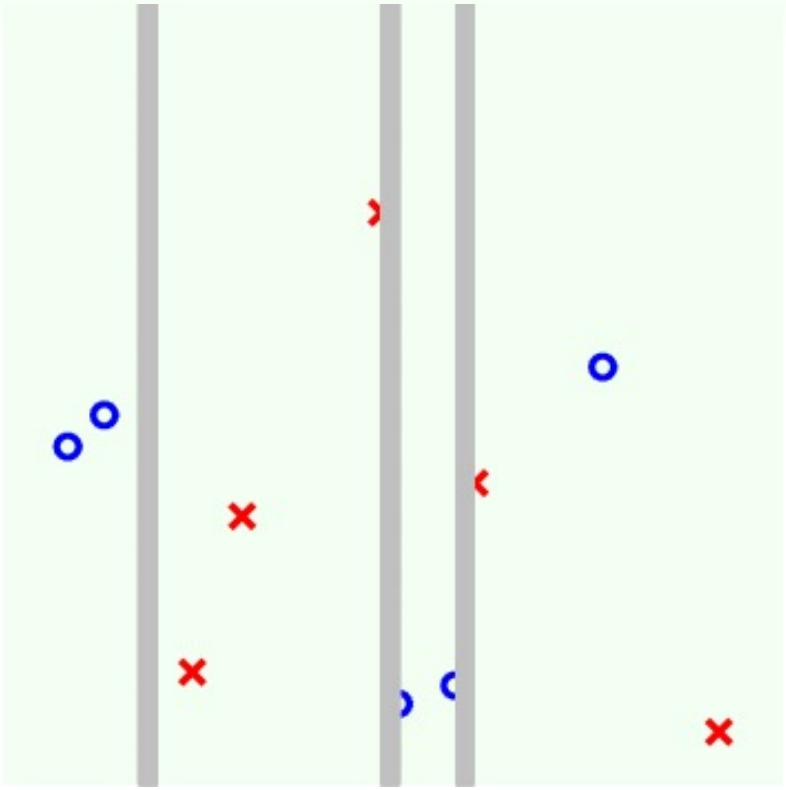

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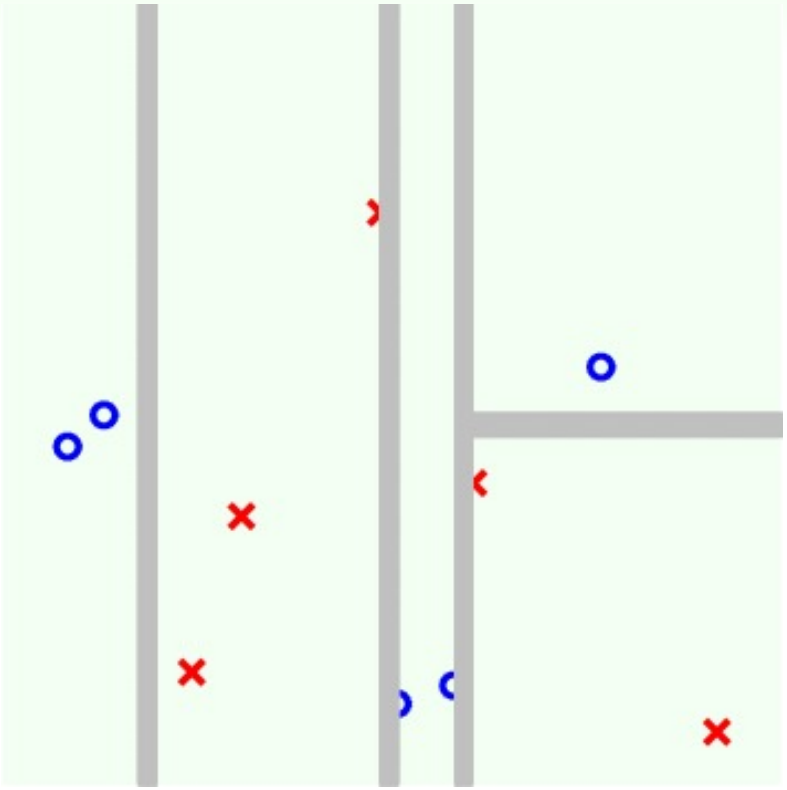

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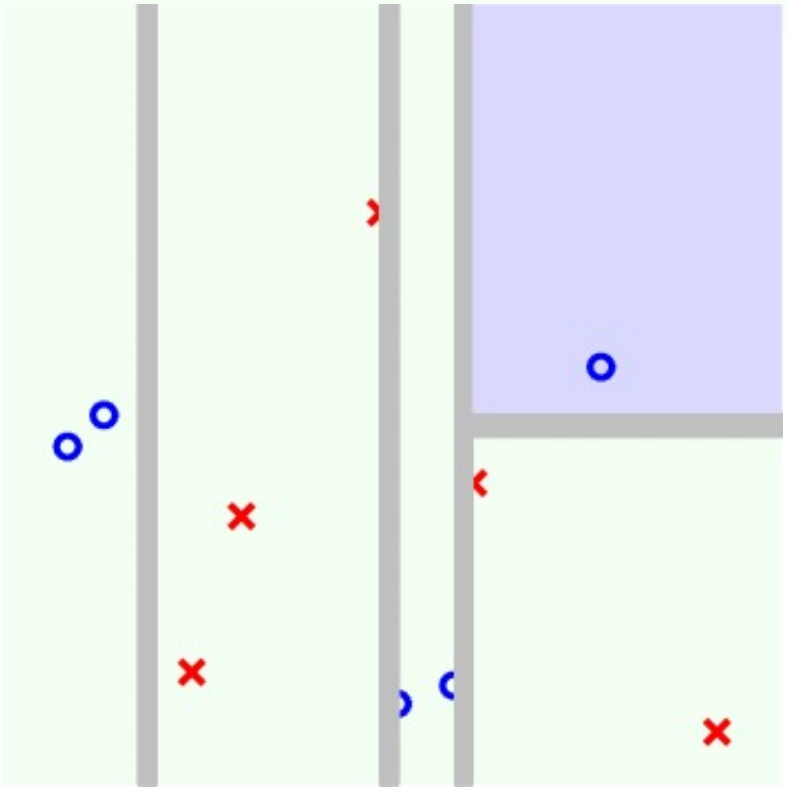

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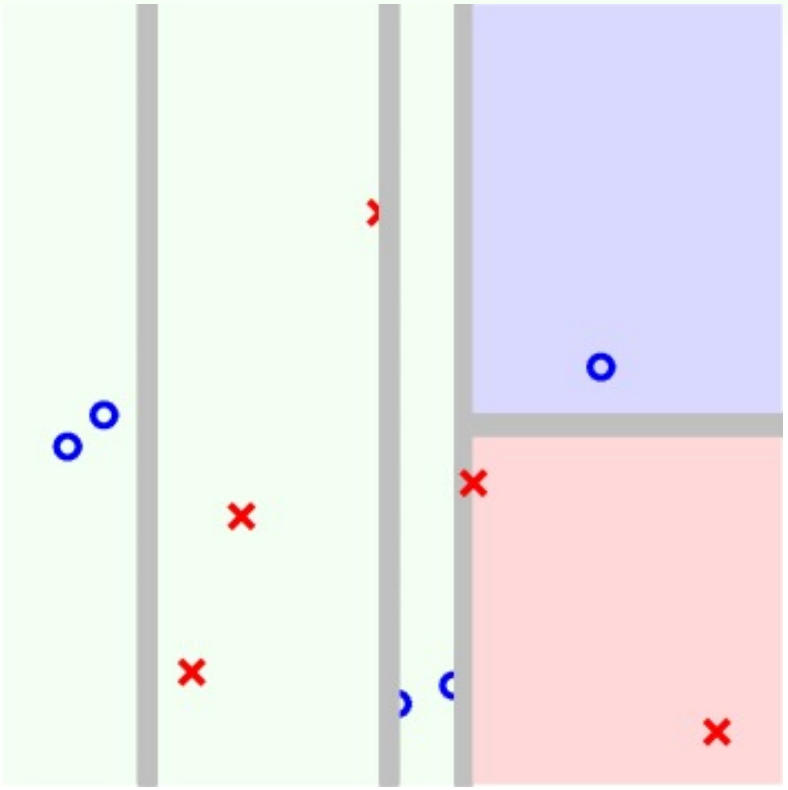

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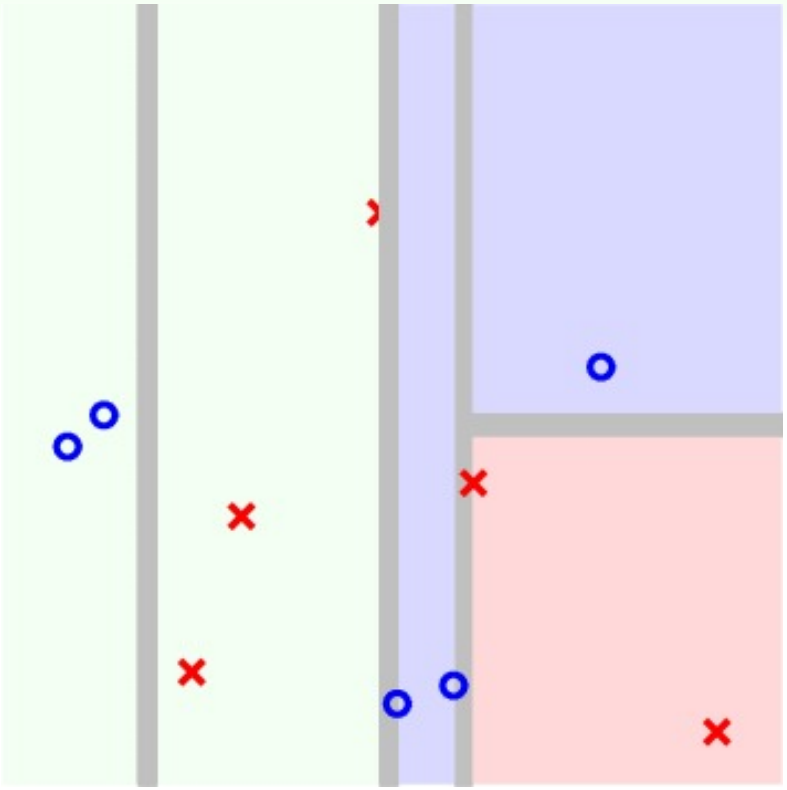

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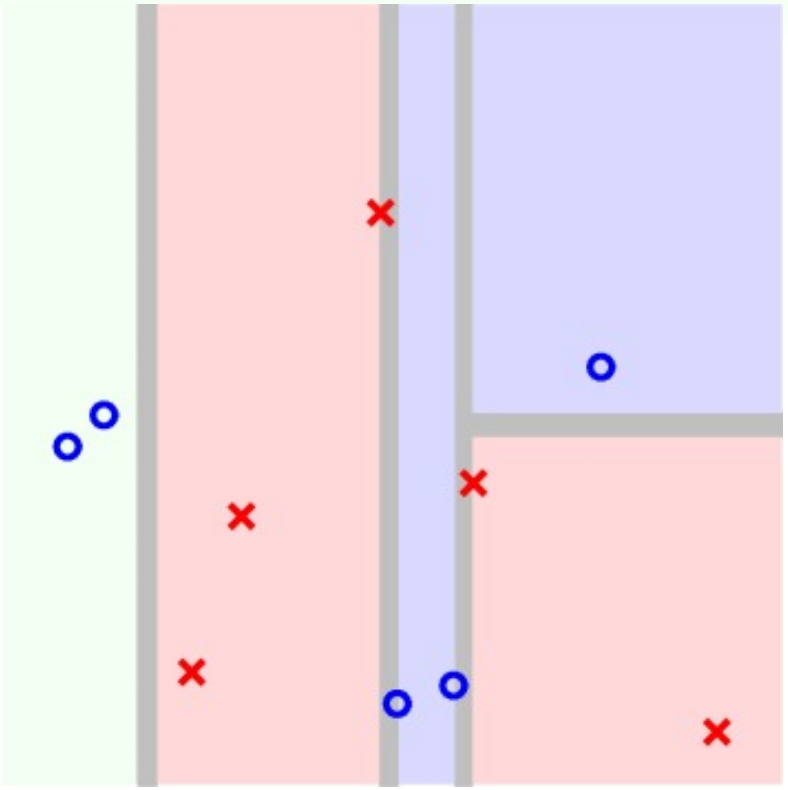

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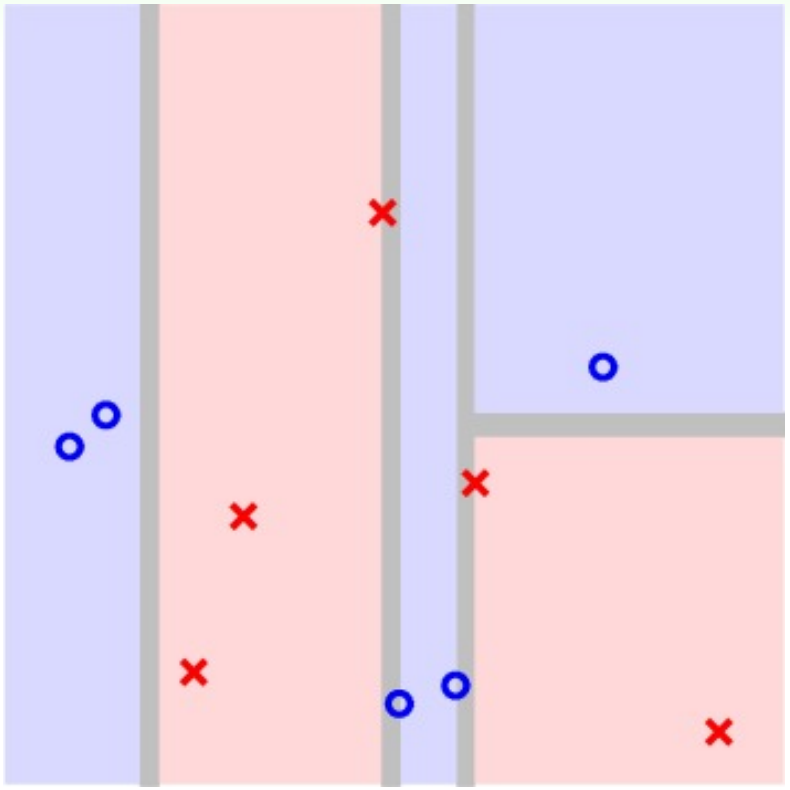

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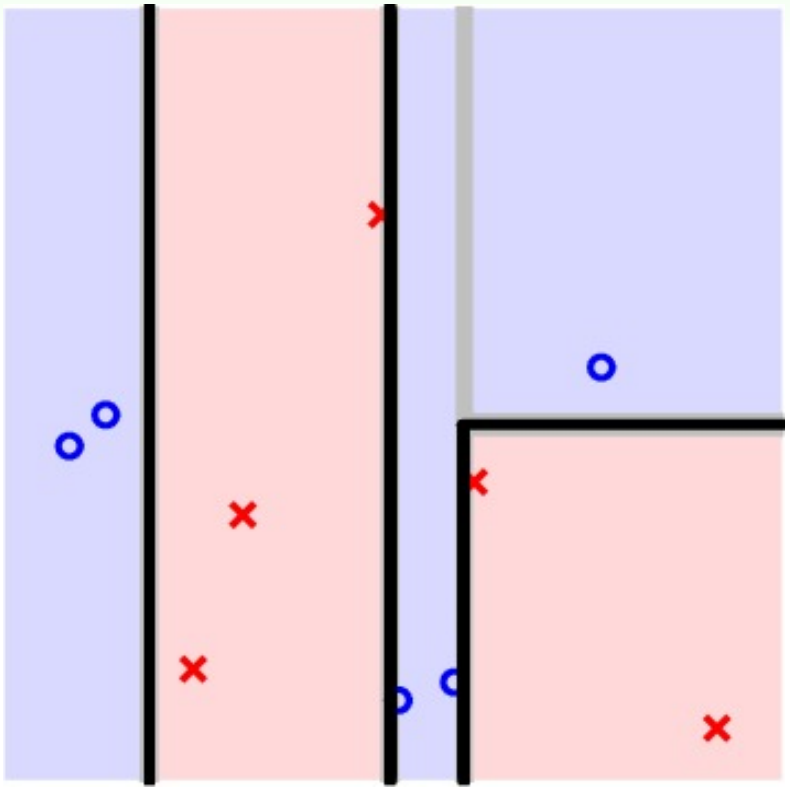
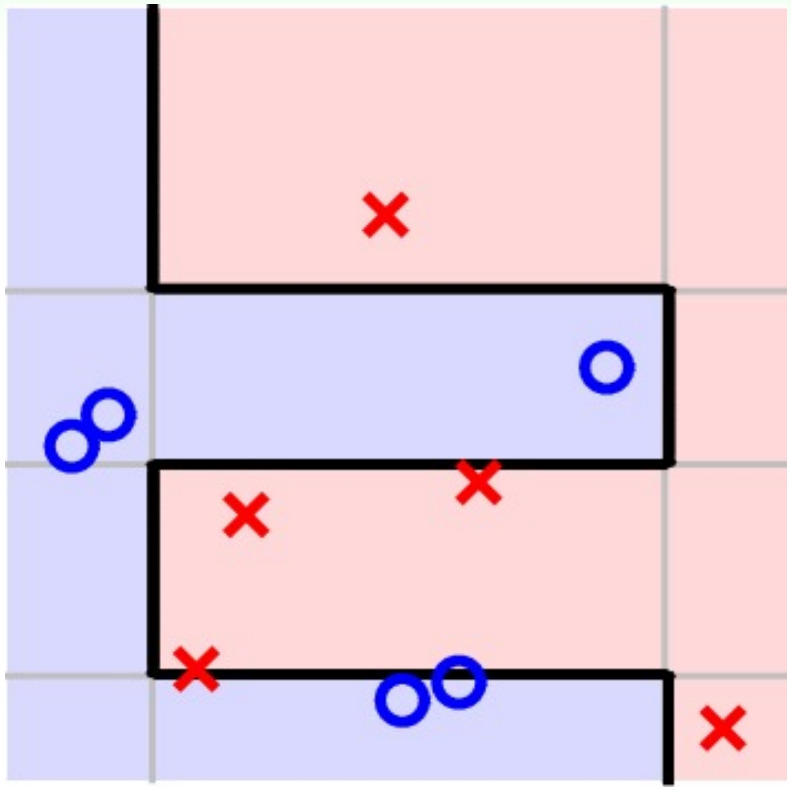


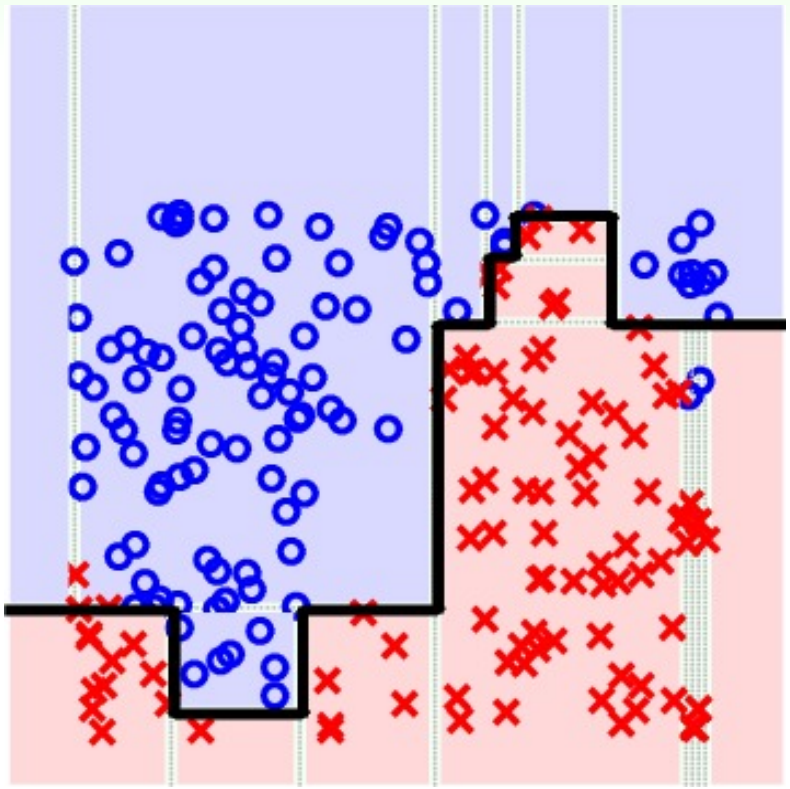
C&RT



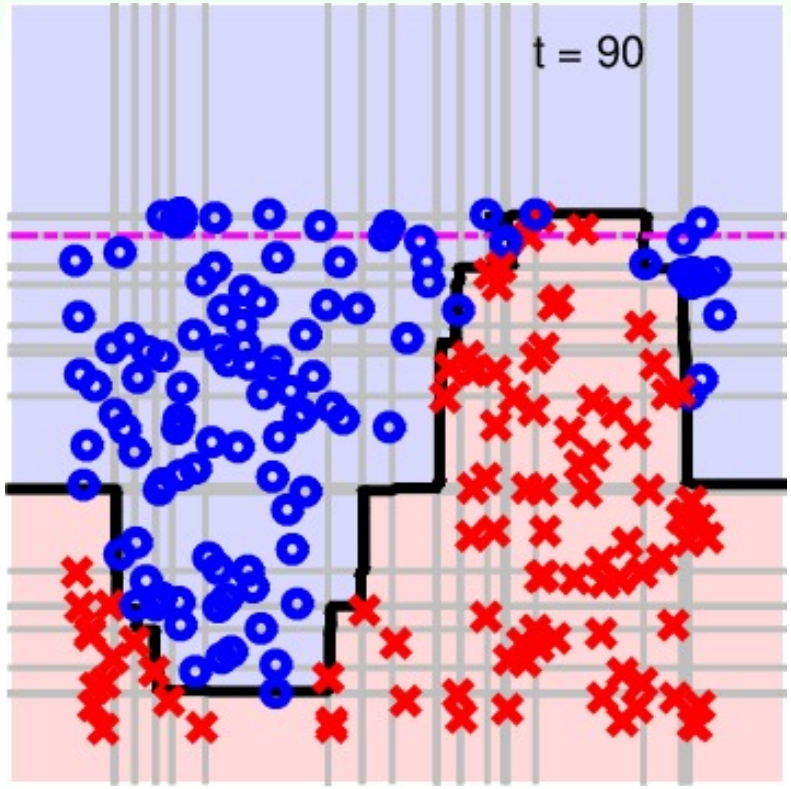
AdaBoost-Stump

C&RT: 'divide-and-conquer'

A Complicated Data Set



C&RT



AdaBoost-Stump

C&RT: even more efficient than AdaBoost-Stump

Practical Specialties of C&RT

- human-explainable
- multiclass easily
- categorical features easily (details omitted)
- missing features easily (details omitted)
- efficient non-linear training (and testing)

—almost no other learning model share all such specialties, except for **other decision trees**

another popular decision tree algorithm:
C4.5, with different **choices of heuristics**

Questions?

Recall: Bagging and Decision Tree

Bagging

function Bag($\mathcal{D}, \mathcal{A}$)
For $t = 1, 2, \ldots, T$

1. request size-N' data $\tilde{\mathcal{D}}_t$ by bootstrapping with $\mathcal{D}$
2. obtain base g_t by $\mathcal{A}(\tilde{\mathcal{D}}_t)$

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

—reduces variance
by voting/averaging

Decision Tree

function DTree($\mathcal{D}$)
if termination return base g_t
else

1. learn $b(\mathbf{x})$ and split $\mathcal{D}$ to $\mathcal{D}_c$ by $b(\mathbf{x})$
2. build $G_c \leftarrow \text{DTree}(\mathcal{D}_c)$
3. return $G(\mathbf{x}) = \sum_{c=1}^{C} [\![b(\mathbf{x}) = c]\!] \, G_c(\mathbf{x})$

—large variance
especially if fully-grown

putting them together?
(i.e. aggregation of aggregation :-))

Random Forest (RF)

random forest (RF) = bagging + fully-grown C&RT decision tree

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 DTree($\tilde{\mathcal{D}}_t$)

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

function DTree($\mathcal{D}$)
if termination return base g_t
else

1. learn $b(\mathbf{x})$ and split $\mathcal{D}$ to $\mathcal{D}_c$ by $b(\mathbf{x})$
2. build $G_c \leftarrow \text{DTree}(\mathcal{D}_c)$
3. return $G(\mathbf{x}) = \sum_{c=1}^{C} [\![b(\mathbf{x}) = c]\!] \, G_c(\mathbf{x})$

- highly **parallel**/**efficient** to learn
- **inherit pros** of C&RT
- **eliminate cons** of fully-grown tree

Diversifying by Feature Expansion

randomly **sample** d' **features** from $\mathbf{x}$: $\Phi(\mathbf{x}) = \mathrm{P} \cdot \mathbf{x}$
with row i of P sampled randomly

- **projection** (combination) with random row $\mathbf{p}_i$ of P: $\phi_i(\mathbf{x}) = \mathbf{p}_i^T \mathbf{x}$
- often consider **low-dimensional** projection:
  only d'' **non-zero** components in $\mathbf{p}_i$
- original RF consider d' random **low-dimensional projections for each** $b(\mathbf{x})$ in C&RT

RF = bagging + random-**combination** C&RT
—randomness everywhere!

Questions?

Bagging Revisited

Bagging

function Bag($\mathcal{D}, \mathcal{A}$)
For $t = 1, 2, \ldots, T$

1. request size-N' data $\tilde{\mathcal{D}}_t$ by bootstrapping with $\mathcal{D}$
2. obtain base g_t by $\mathcal{A}(\tilde{\mathcal{D}}_t)$

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

	g_1	g_2	g_3	$\cdots$	g_T
$(\mathbf{x}_1, y_1)$	$\tilde{\mathcal{D}}_1$	$\star$	$\tilde{\mathcal{D}}_3$		$\tilde{\mathcal{D}}_T$
$(\mathbf{x}_2, y_2)$	$\star$	$\star$	$\tilde{\mathcal{D}}_3$		$\tilde{\mathcal{D}}_T$
$(\mathbf{x}_3, y_3)$	$\star$	$\tilde{\mathcal{D}}_2$	$\star$		$\tilde{\mathcal{D}}_T$
$\cdots$					
$(\mathbf{x}_N, y_N)$	$\tilde{\mathcal{D}}_1$	$\tilde{\mathcal{D}}_2$	$\star$		$\star$

$\star$ in t-th column: not used for obtaining g_t
—called **out-of-bag (OOB) examples** of g_t

Number of OOB Examples

OOB (in $\star$) $\Longleftrightarrow$ not sampled after N' drawings

if $N' = N$

- probability for $(\mathbf{x}_n, y_n)$ to be OOB for g_t: $\left(1 - \frac{1}{N}\right)^N$
- if N large:

$$\left(1 - \frac{1}{N}\right)^N = \frac{1}{\left(\frac{N}{N-1}\right)^N} = \frac{1}{\left(1 + \frac{1}{N-1}\right)^N} \approx \frac{1}{e}$$

OOB size per $g_t \approx \frac{1}{e}N$

OOB versus Validation

OOB

	g_1	g_2	g_3	$\cdots$	g_T
$(\mathbf{x}_1, y_1)$	$\tilde{\mathcal{D}}_1$	$\star$	$\tilde{\mathcal{D}}_3$		$\tilde{\mathcal{D}}_T$
$(\mathbf{x}_2, y_2)$	$\star$	$\star$	$\tilde{\mathcal{D}}_3$		$\tilde{\mathcal{D}}_T$
$(\mathbf{x}_3, y_3)$	$\star$	$\tilde{\mathcal{D}}_2$	$\star$		$\tilde{\mathcal{D}}_T$
$\cdots$					
$(\mathbf{x}_N, y_N)$	$\tilde{\mathcal{D}}_1$	$\star$	$\star$		$\star$

Validation

g_1^-	g_2^-	$\cdots$	g_M^-
$\mathcal{D}_{\text{train}}$	$\mathcal{D}_{\text{train}}$		$\mathcal{D}_{\text{train}}$
$\mathcal{D}_{\text{val}}$	$\mathcal{D}_{\text{val}}$		$\mathcal{D}_{\text{val}}$
$\mathcal{D}_{\text{val}}$	$\mathcal{D}_{\text{val}}$		$\mathcal{D}_{\text{val}}$
$\mathcal{D}_{\text{train}}$	$\mathcal{D}_{\text{train}}$		$\mathcal{D}_{\text{train}}$

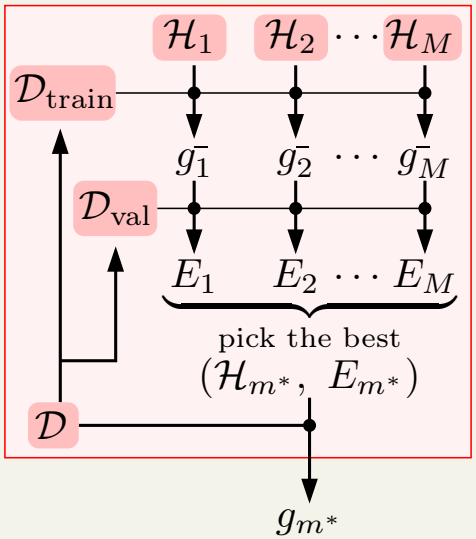
- $\star$ like $\mathcal{D}_{\text{val}}$: 'enough' random examples unused during training
- use $\star$ to validate g_t? easy, but **rarely needed**
- use $\star$ to validate G? $E_{\text{oob}}(G) = \frac{1}{N}\sum_{n=1}^{N} \text{err}(y_n, G_n^-(\mathbf{x}_n))$, with G_n^- contains only trees that $\mathbf{x}_n$ is OOB of,
  such as $G_N^-(\mathbf{x}) = \text{average}(g_2, g_3, g_T)$

E_{oob}: self-validation of bagging/RF

Model Selection by OOB Error

Previously: by Best E_{val}

$$g_{m^*} = \mathcal{A}_{m^*}(\mathcal{D})$$
$$m^* = \underset{1 \le m \le M}{\text{argmin}}\ E_m$$
$$E_m = E_{\text{val}}(\mathcal{A}_m(\mathcal{D}_{\text{train}}))$$



RF: by Best E_{oob}

$$G_{m^*} = \text{RF}_{m^*}(\mathcal{D})$$
$$m^* = \underset{1 \le m \le M}{\text{argmin}}\ E_m$$
$$E_m = E_{\text{oob}}(\text{RF}_m(\mathcal{D}))$$

- use E_{oob} for self-validation —of RF **parameters** such as d''
- no re-training needed

E_{oob} often **accurate** in practice

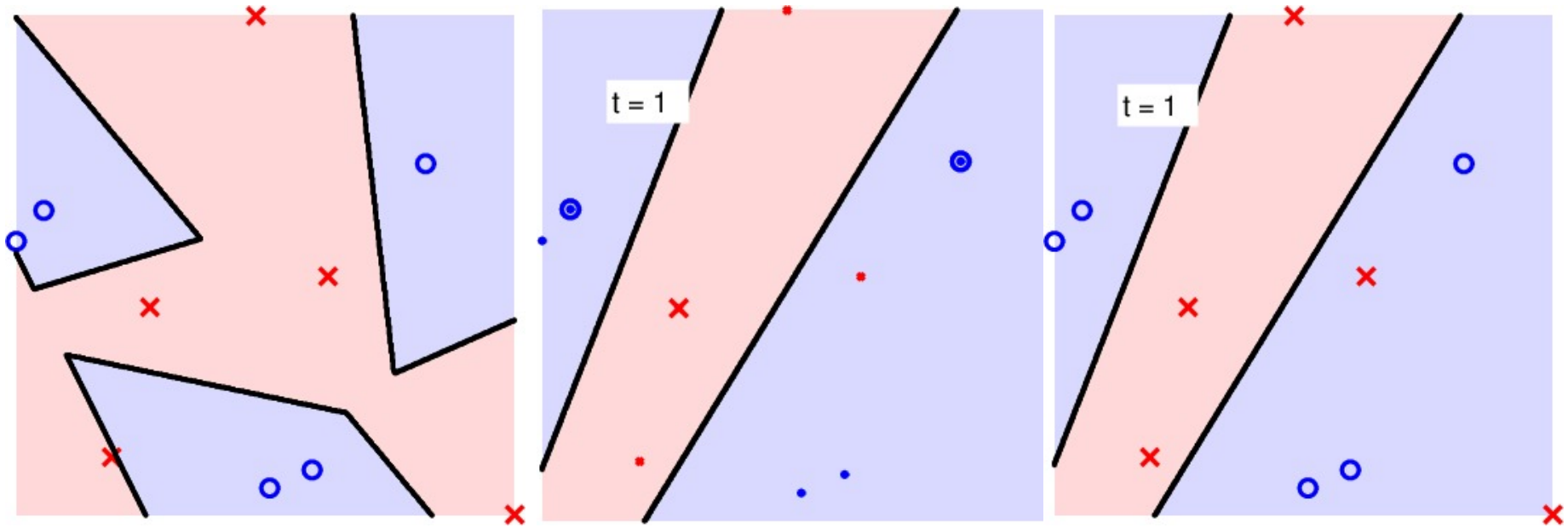
Questions?

A Simple Data Set

$g_{\text{C\&RT}}$ with random combination

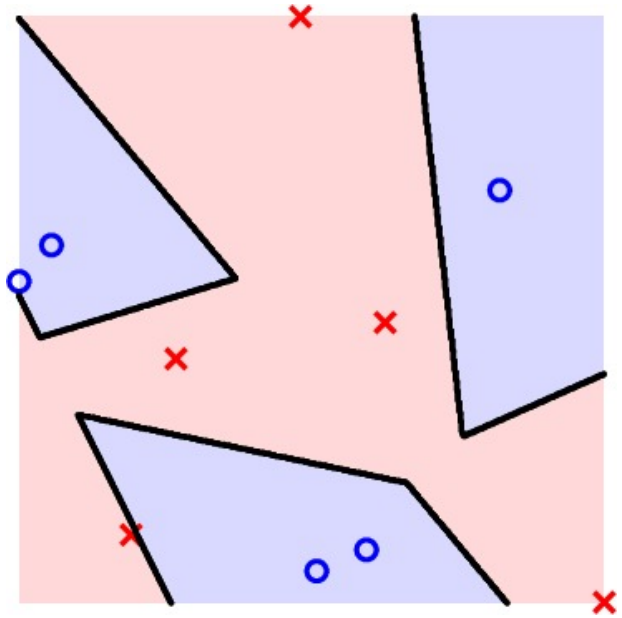
g_t $(N' = N/2)$

G with first t trees

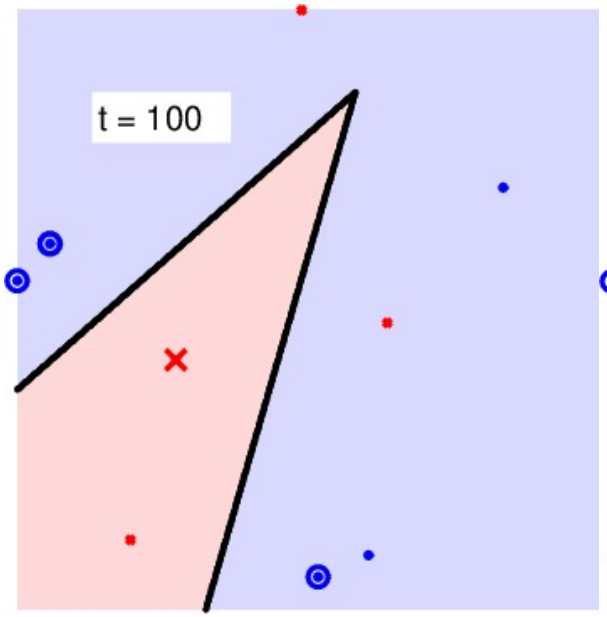


A Simple Data Set

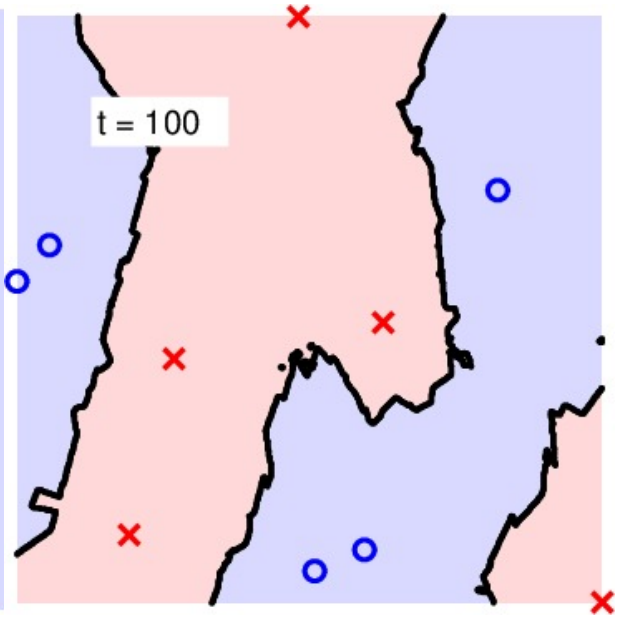
$g_{\text{C\&RT}}$ with random combination



g_t $(N' = N/2)$



G with first t trees

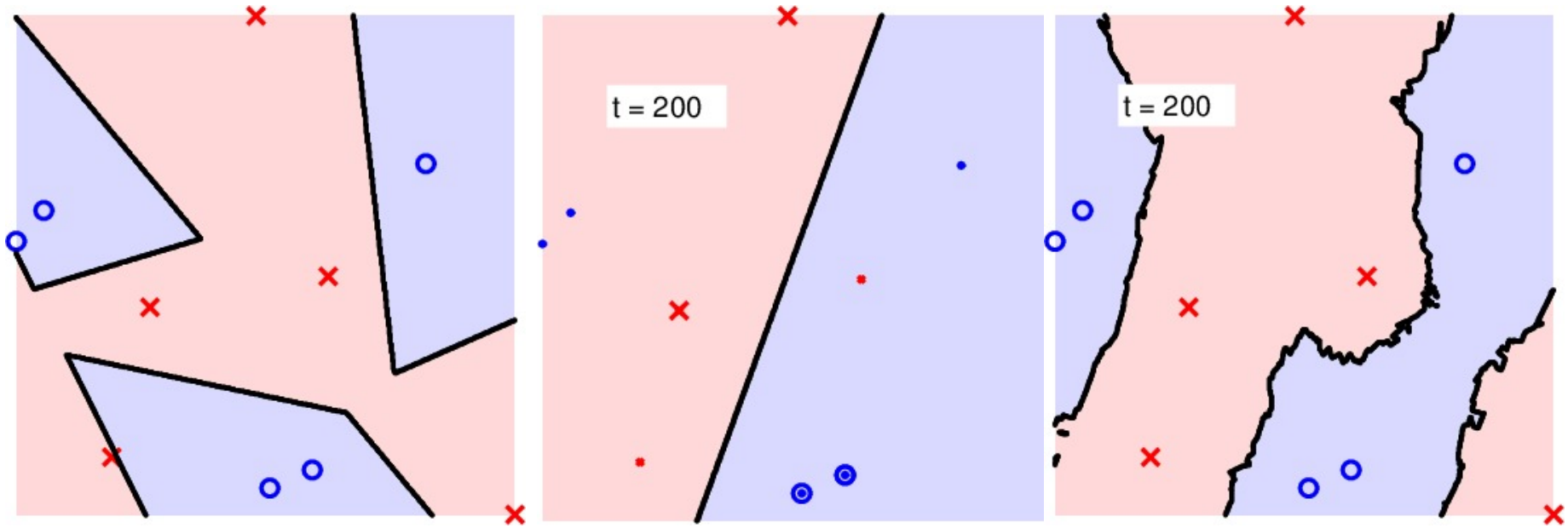


A Simple Data Set

$g_{\text{C\&RT}}$ with random combination

g_t $(N' = N/2)$

G with first t trees

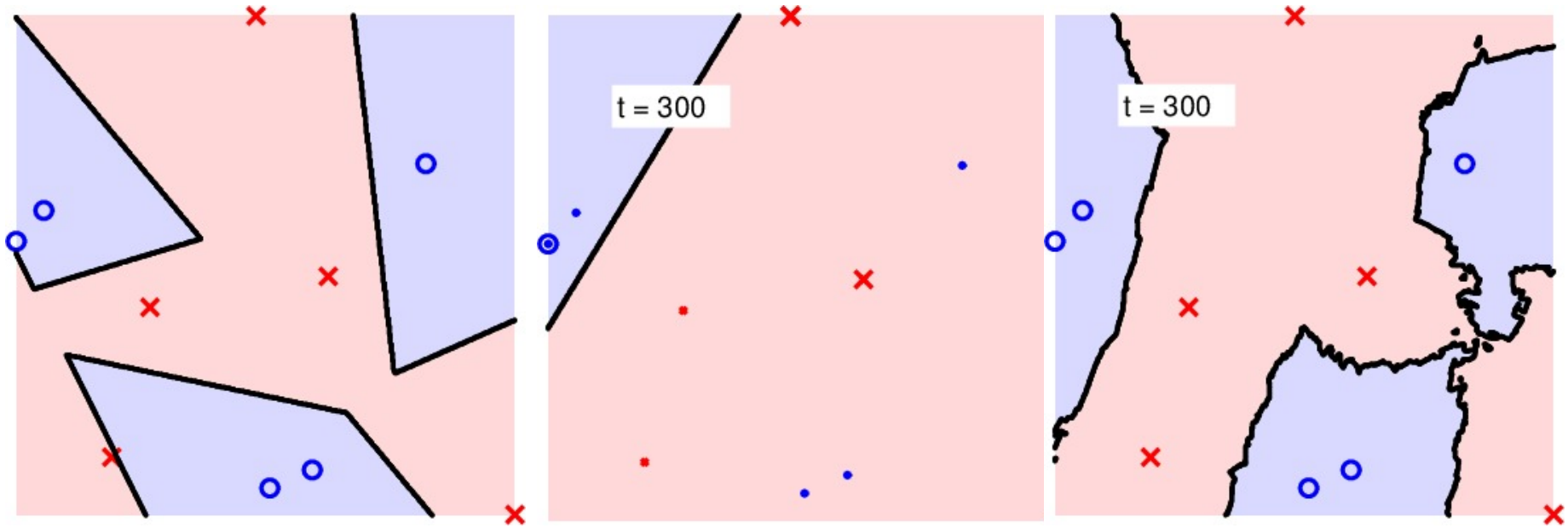


A Simple Data Set

$g_{\text{C\&RT}}$ with random combination

g_t $(N' = N/2)$

G with first t trees



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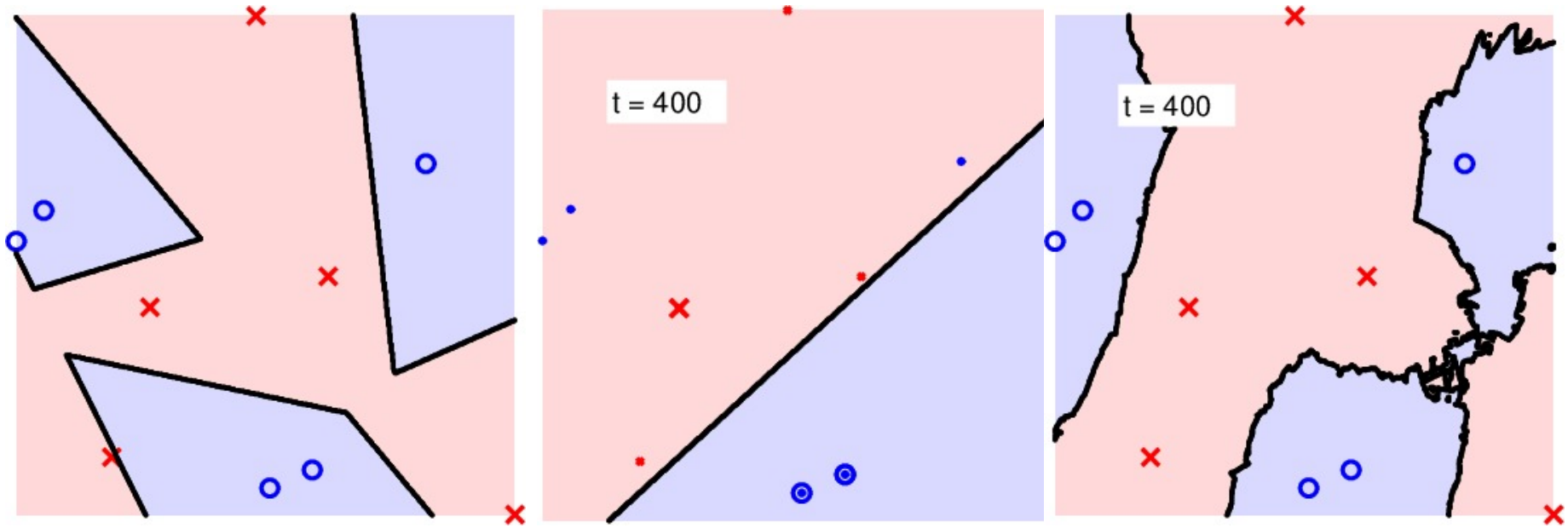

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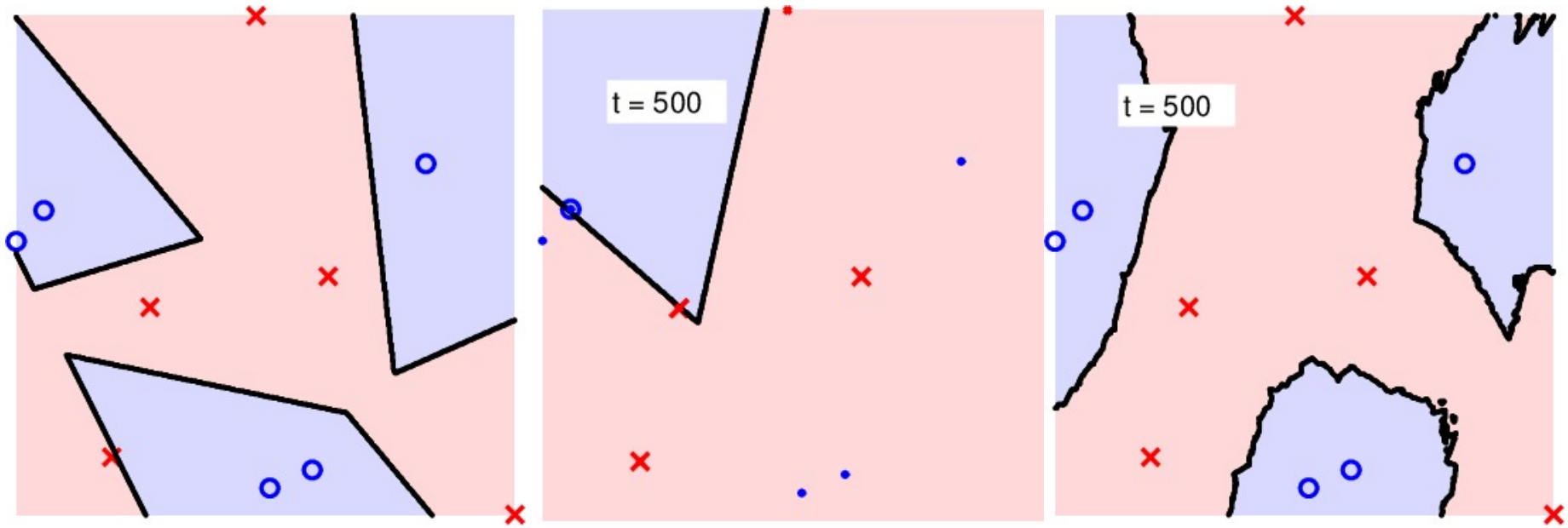

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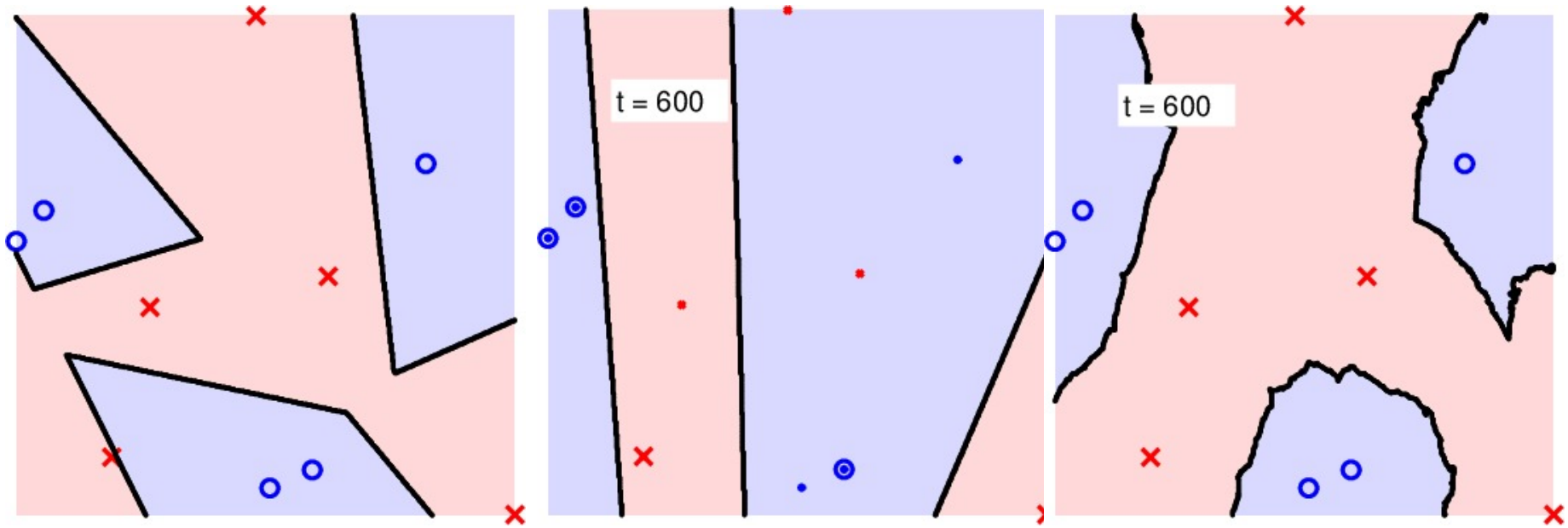

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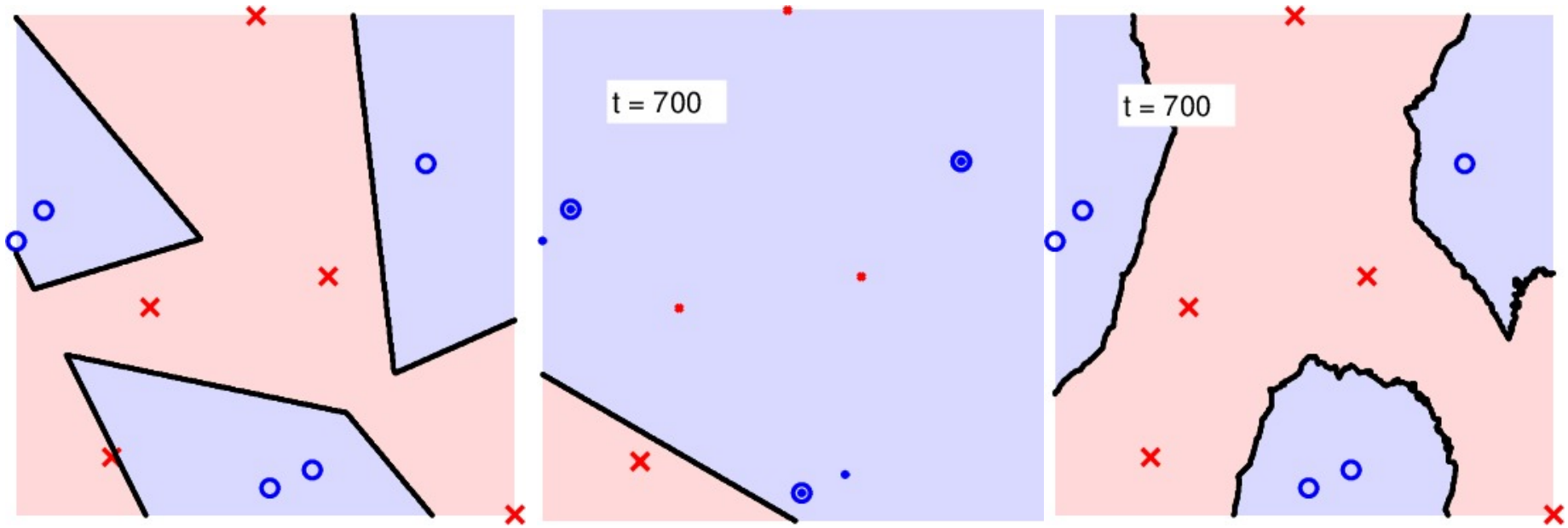

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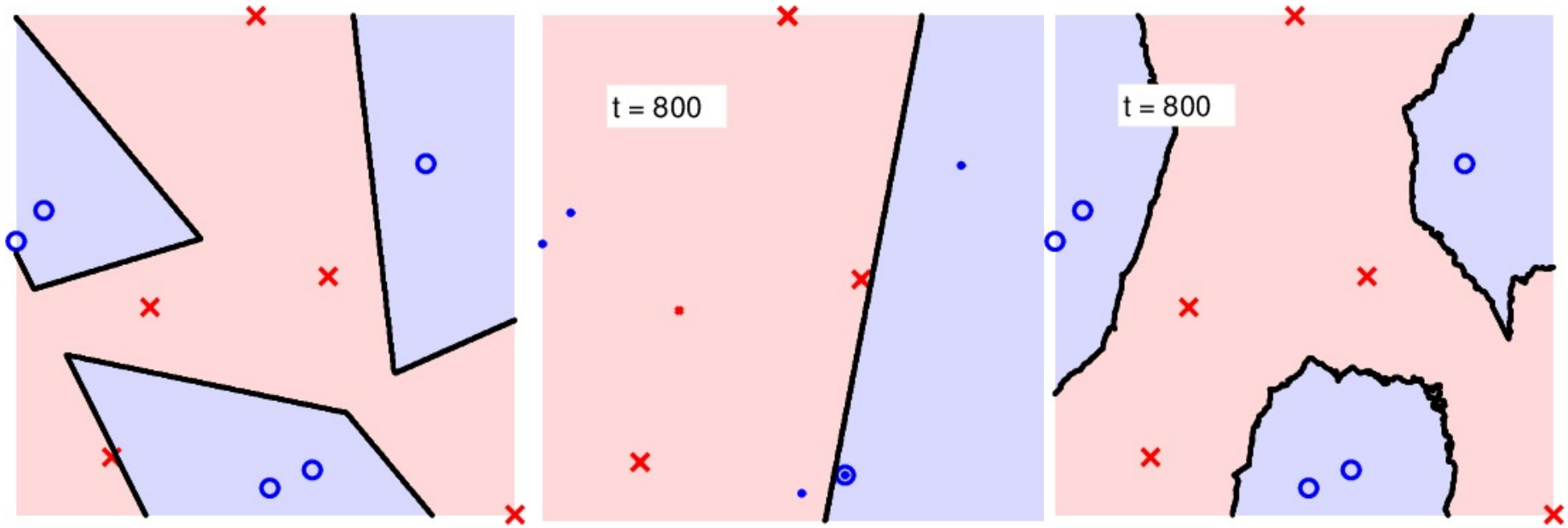

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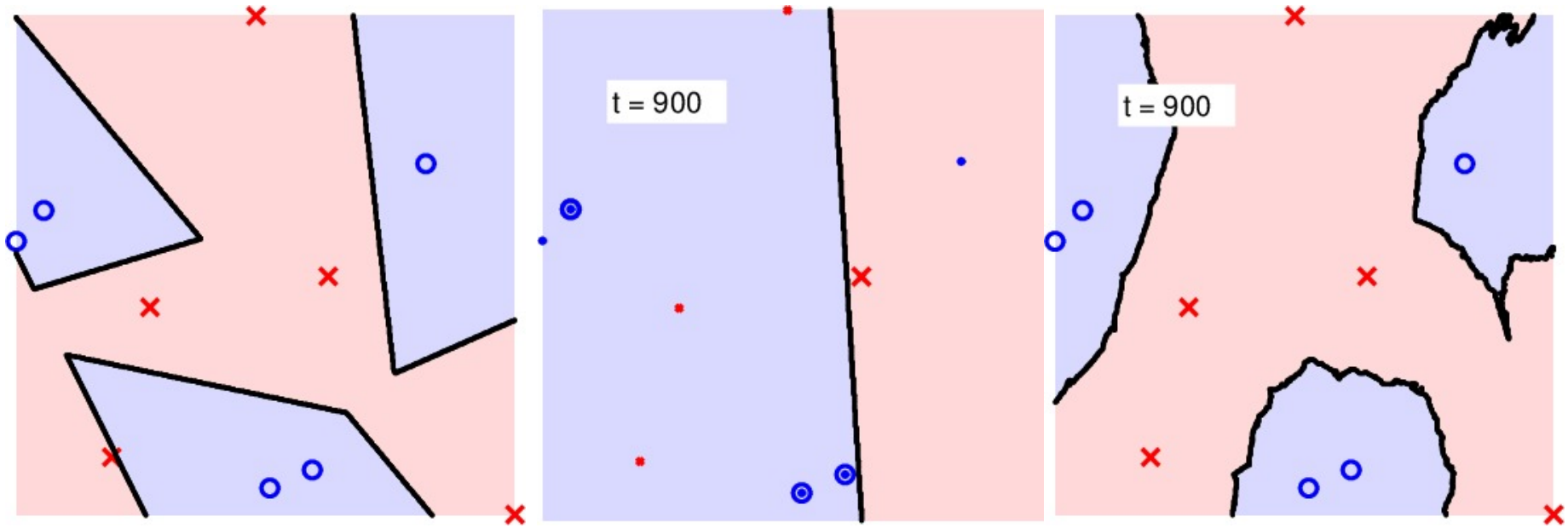

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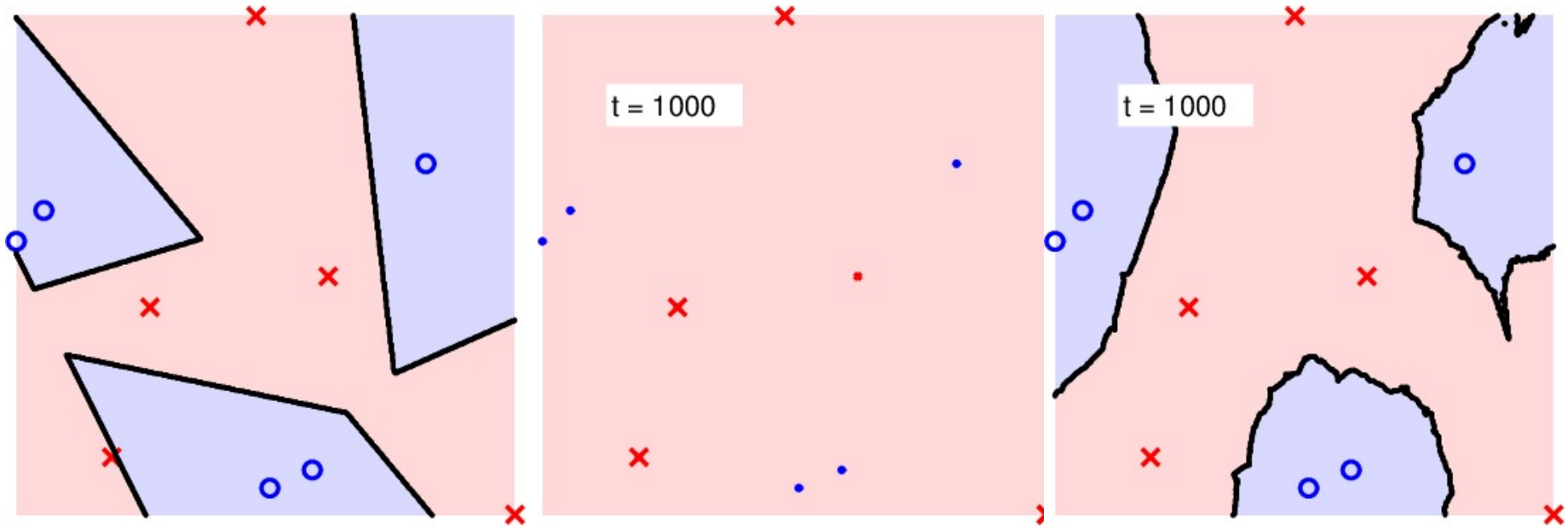
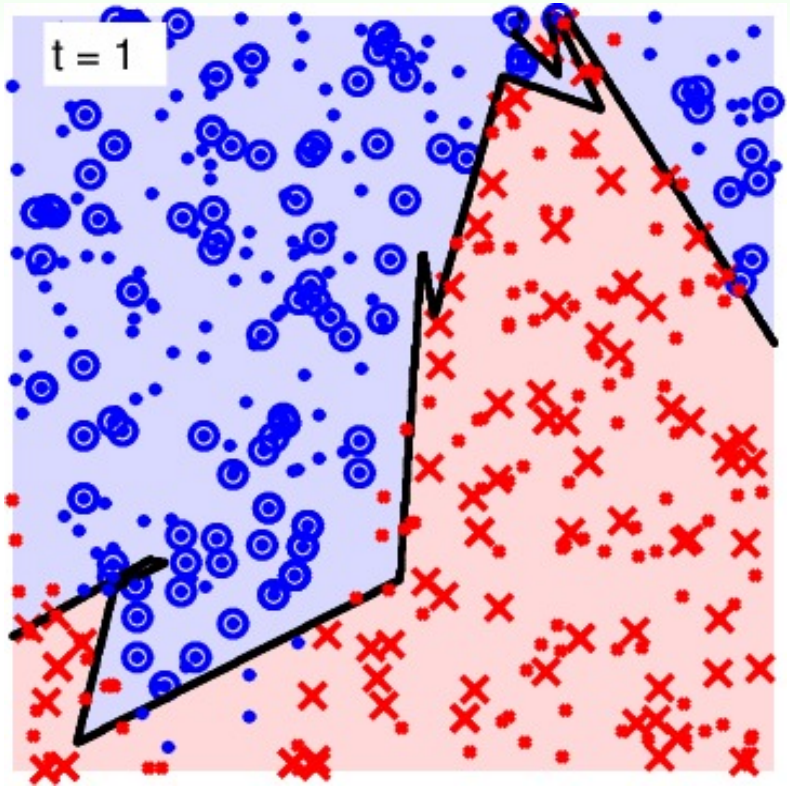


'smooth' and large-margin-like boundary with many trees

A Complicated Data Set

g_t $(N' = N/2)$



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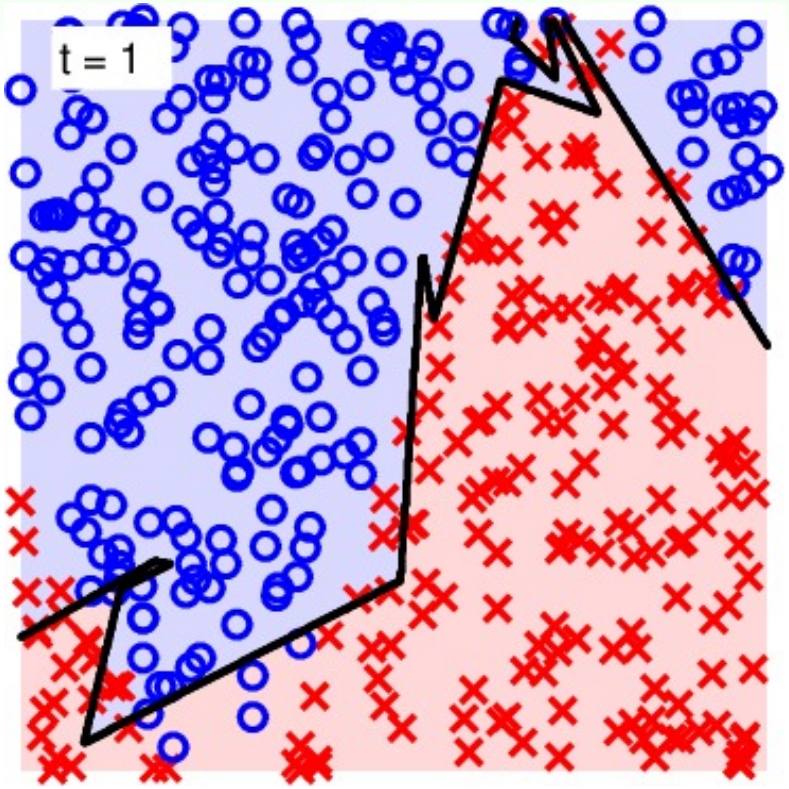

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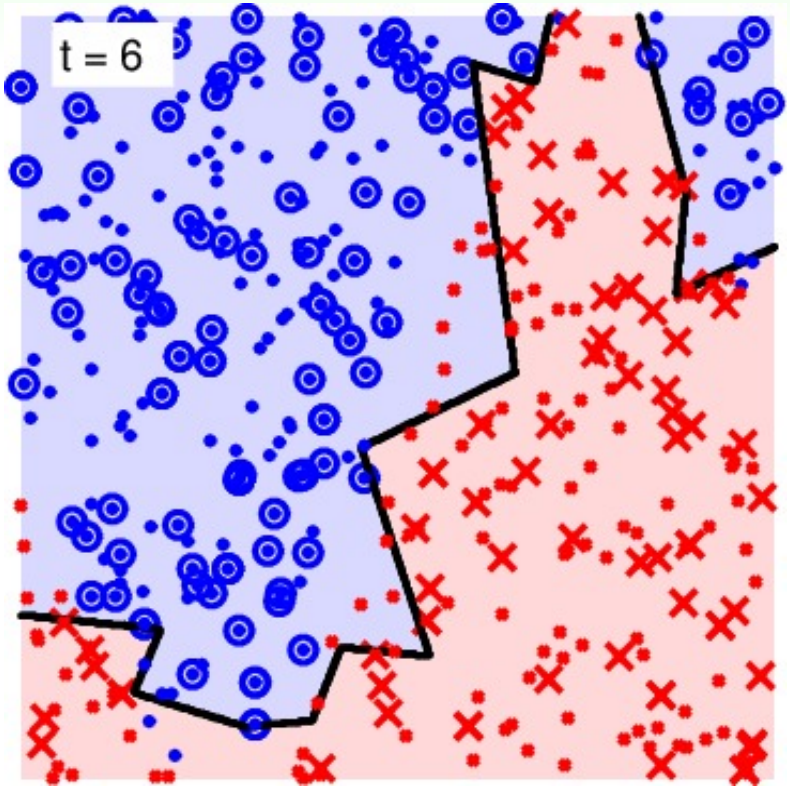

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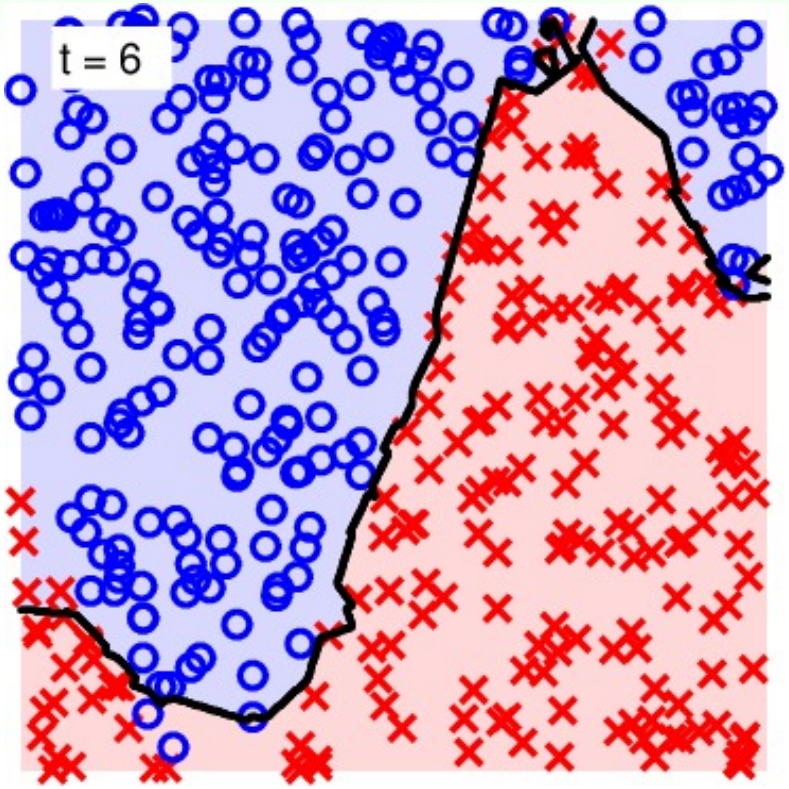
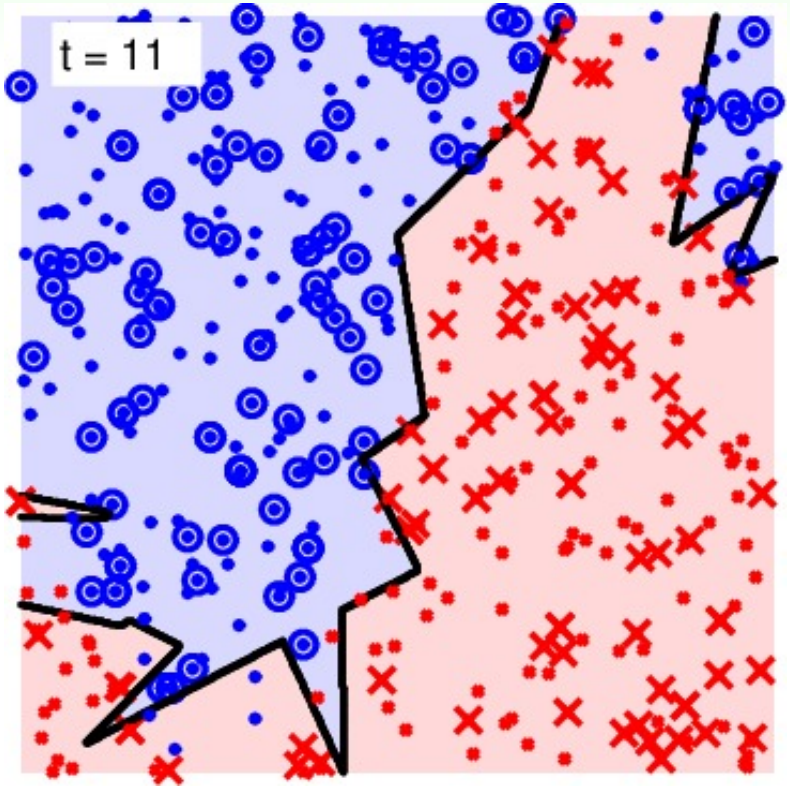


A Complicated Data Set

g_t ($N' = N/2$)



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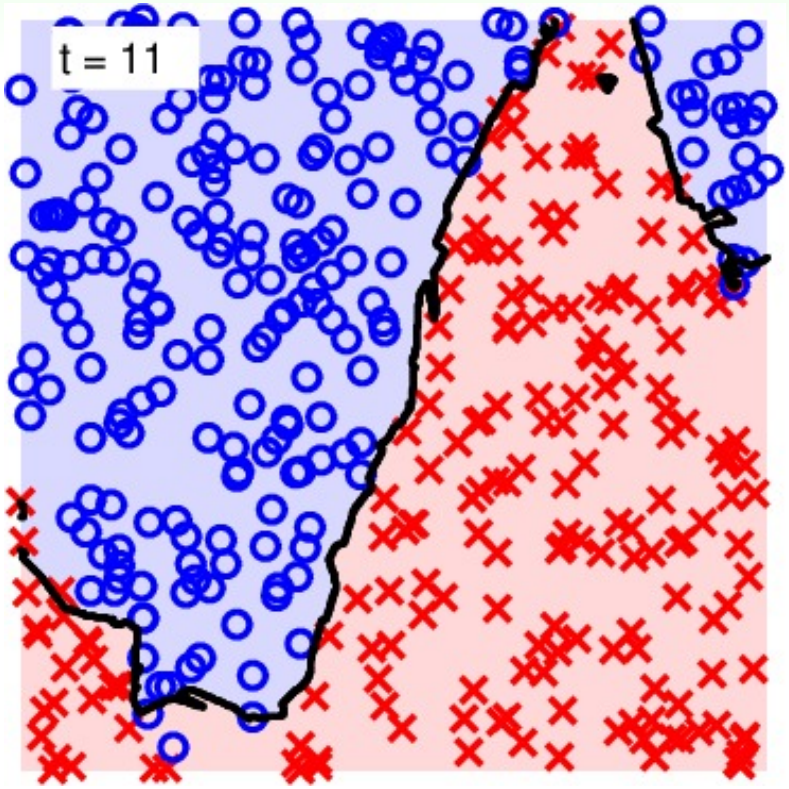

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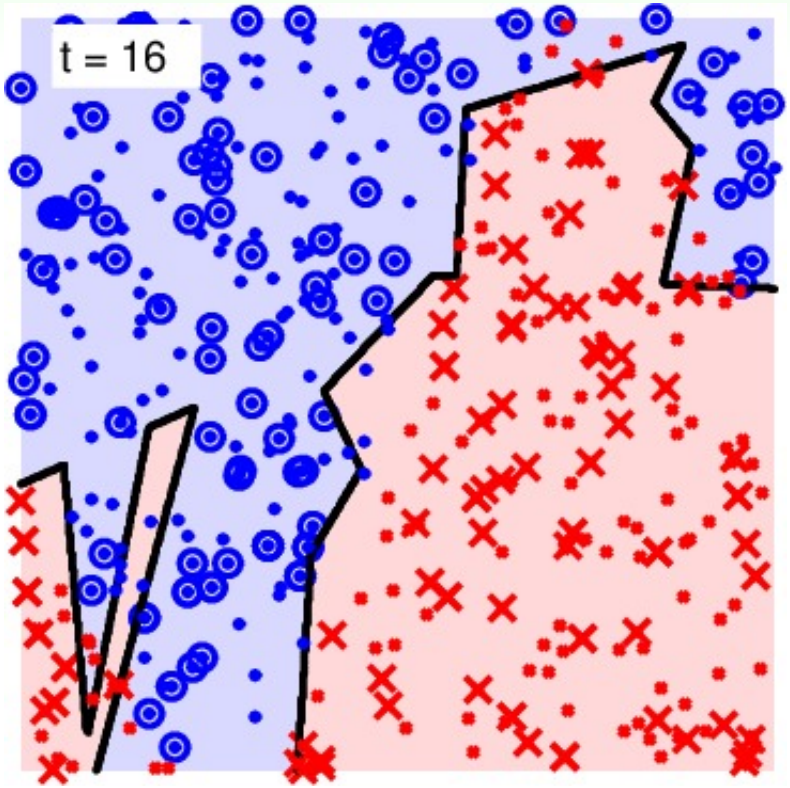

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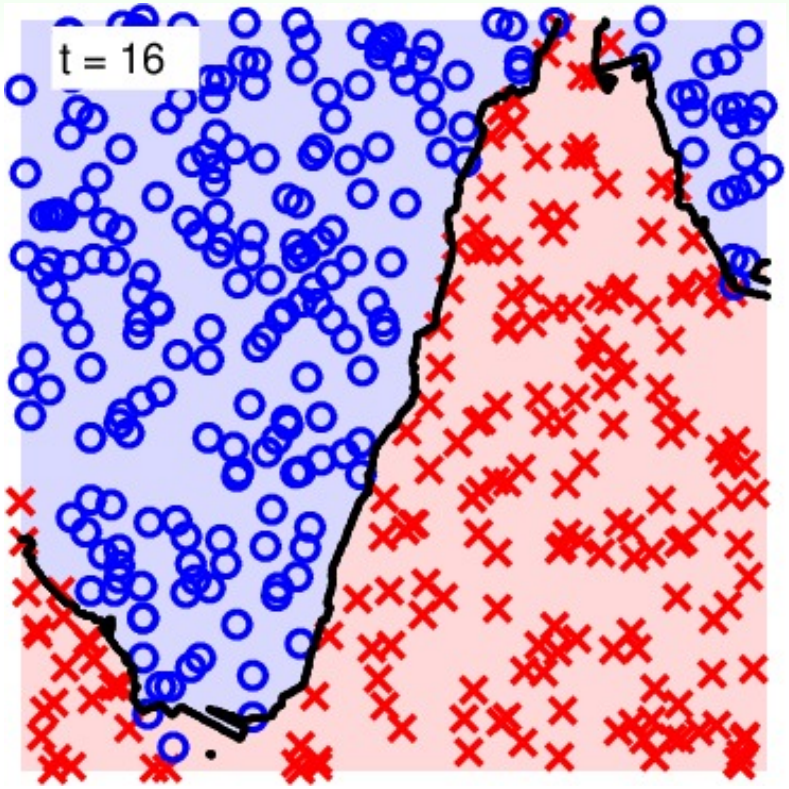

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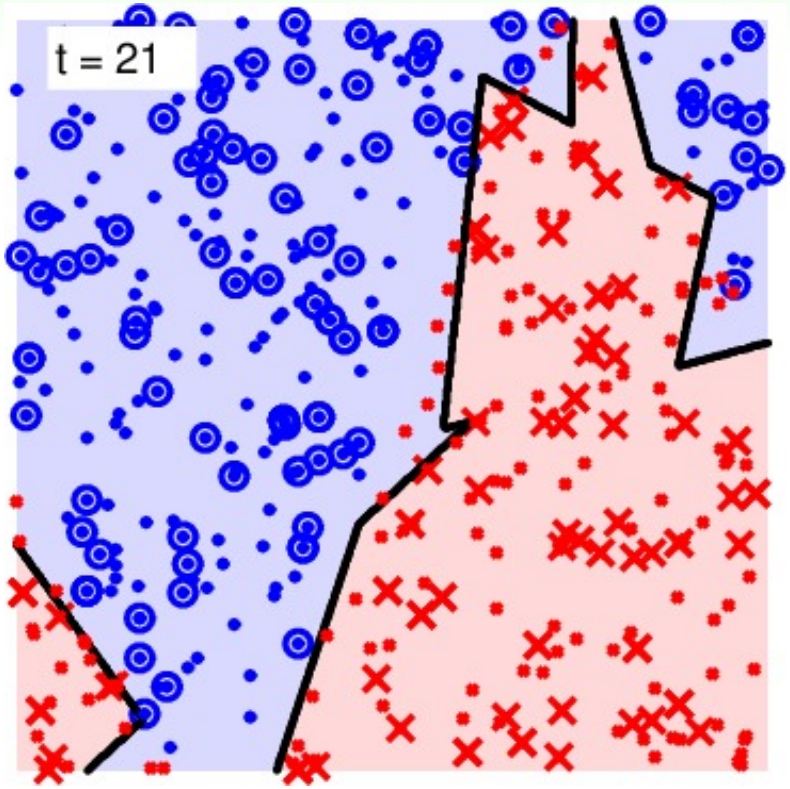

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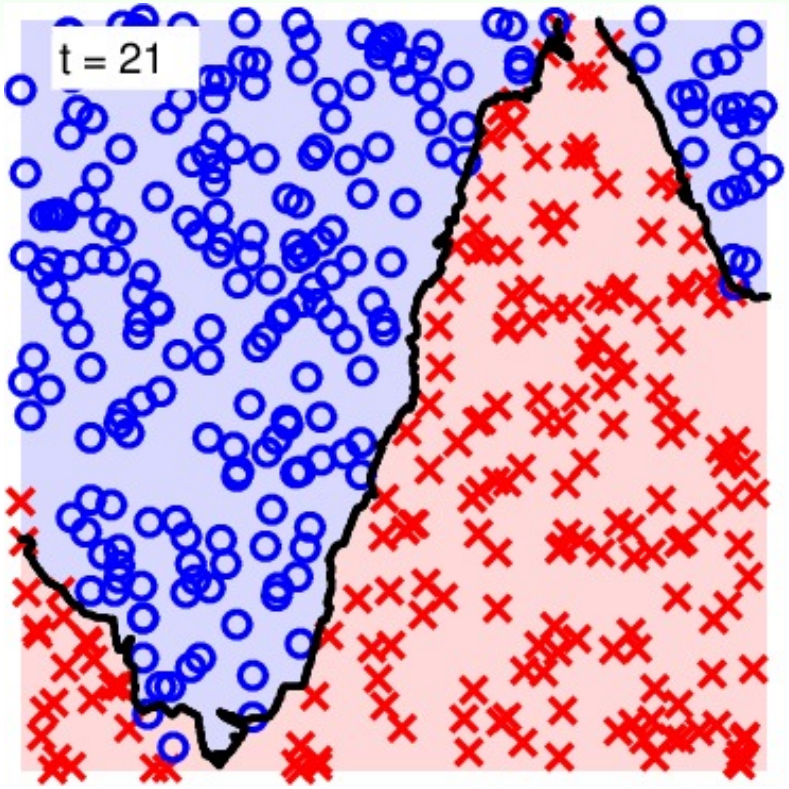
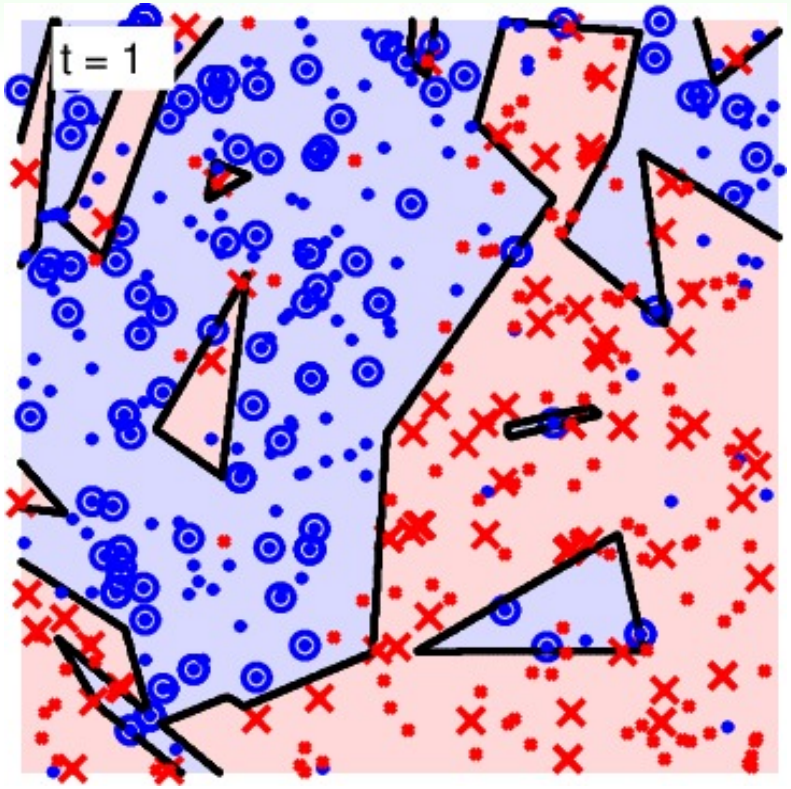


'easy yet robust' nonlinear model

A Complicated and Noisy Data Set

g_t ($N' = N/2$)



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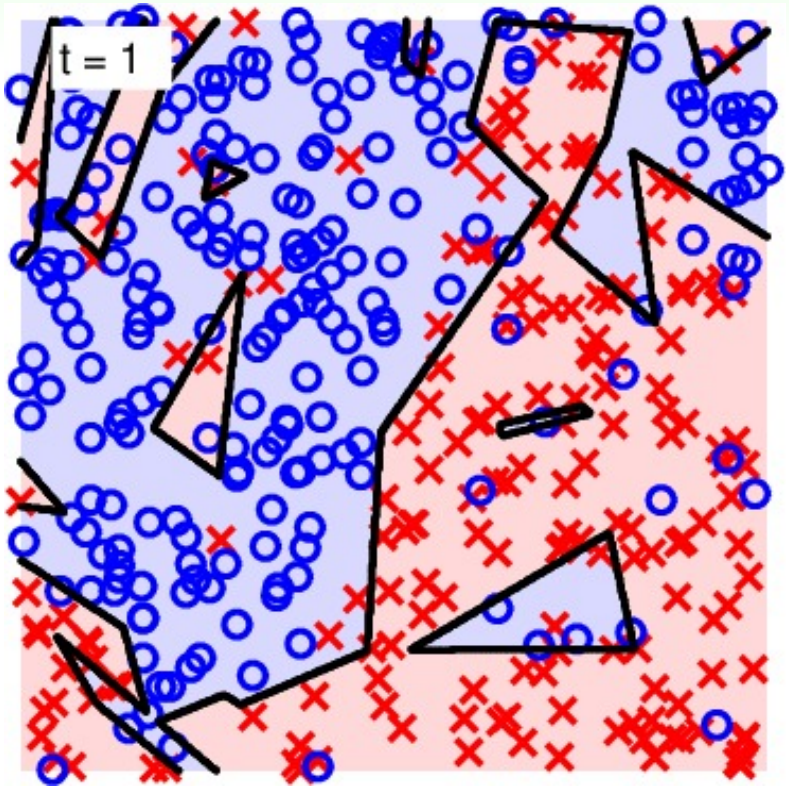

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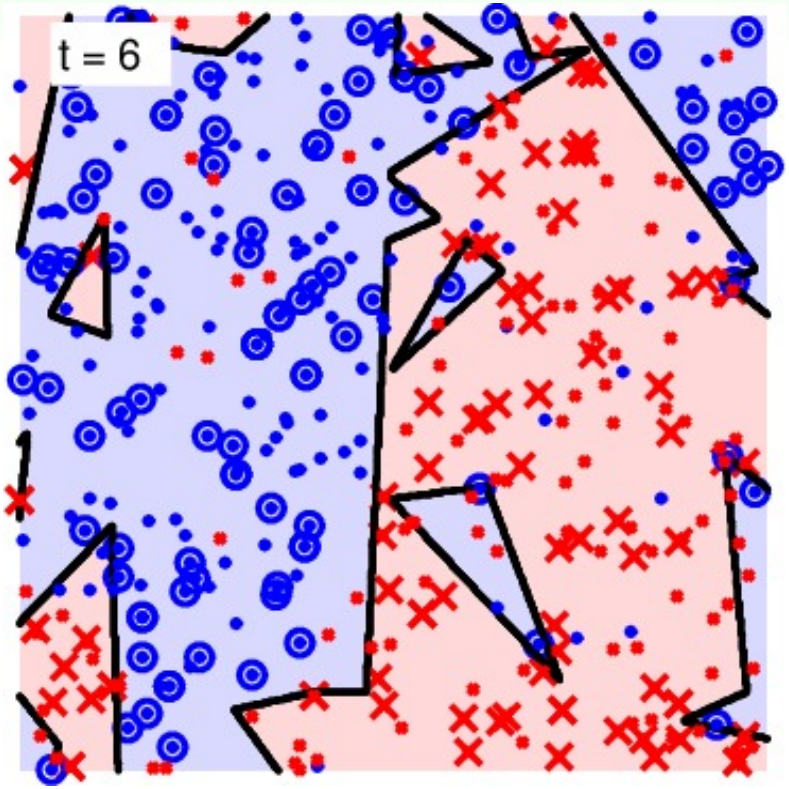

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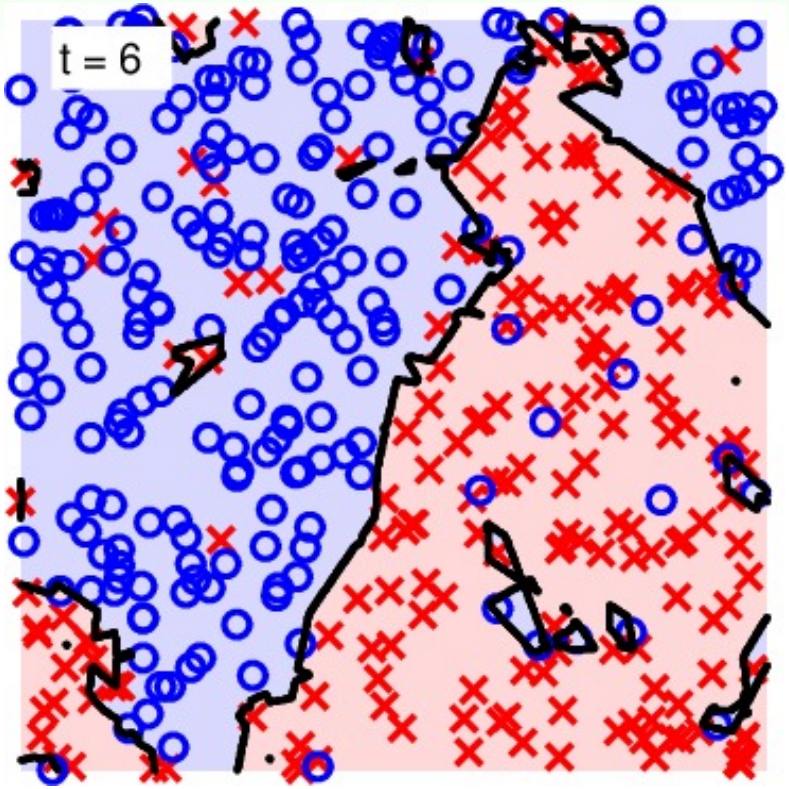

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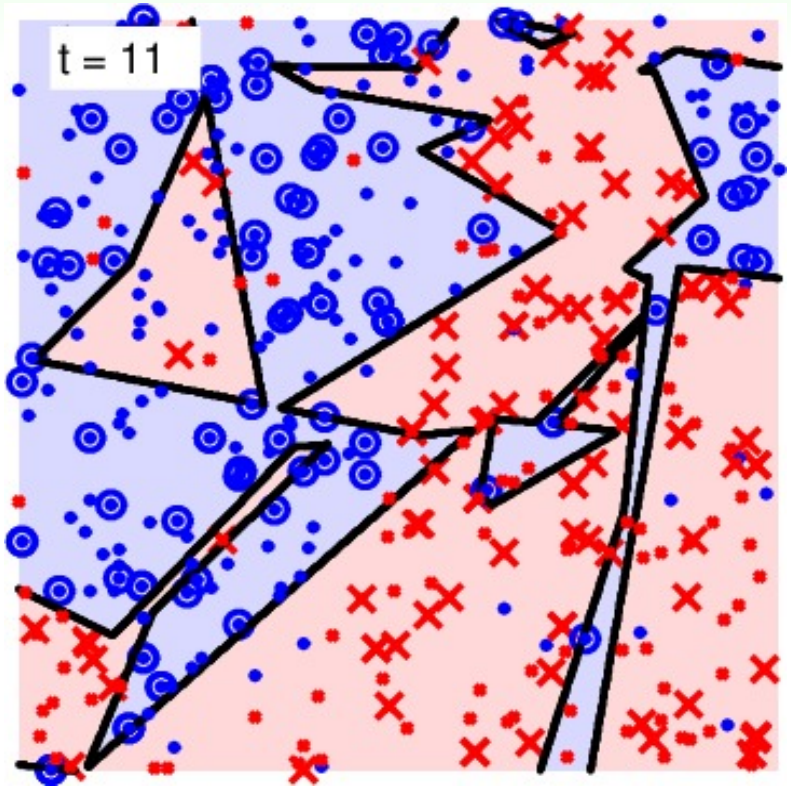

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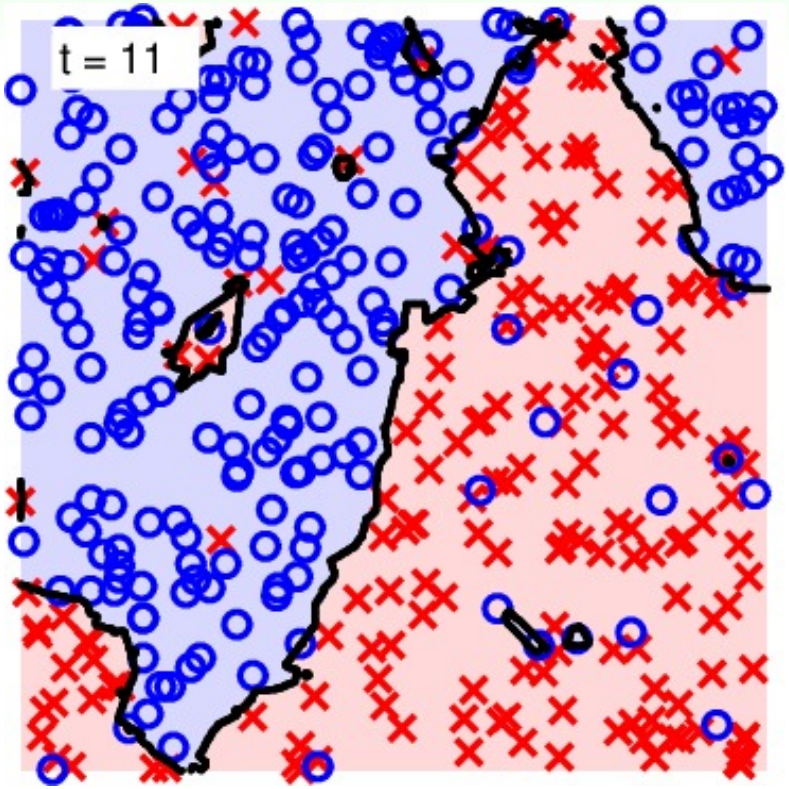

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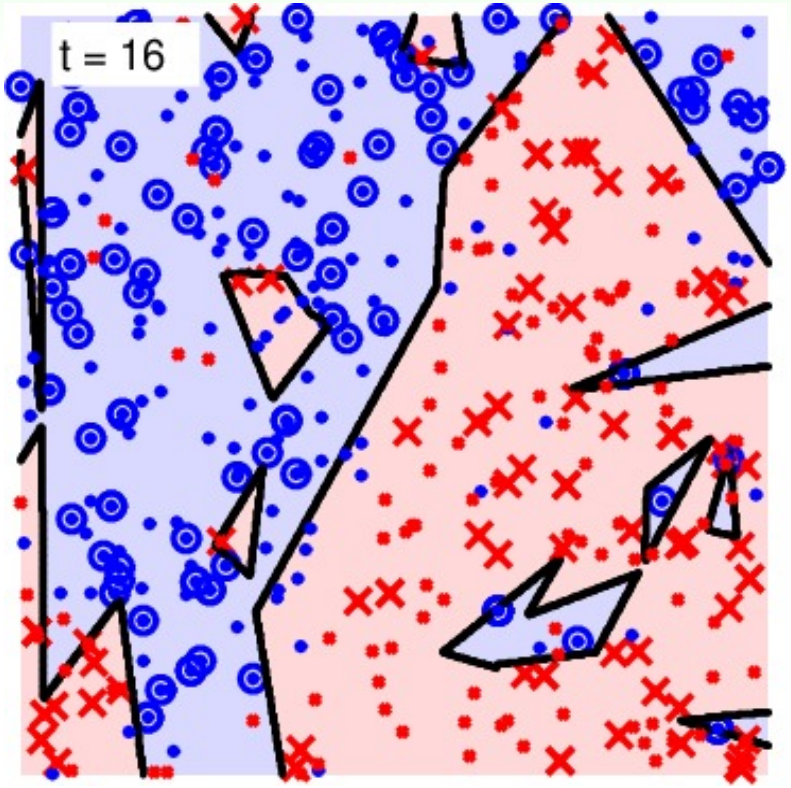

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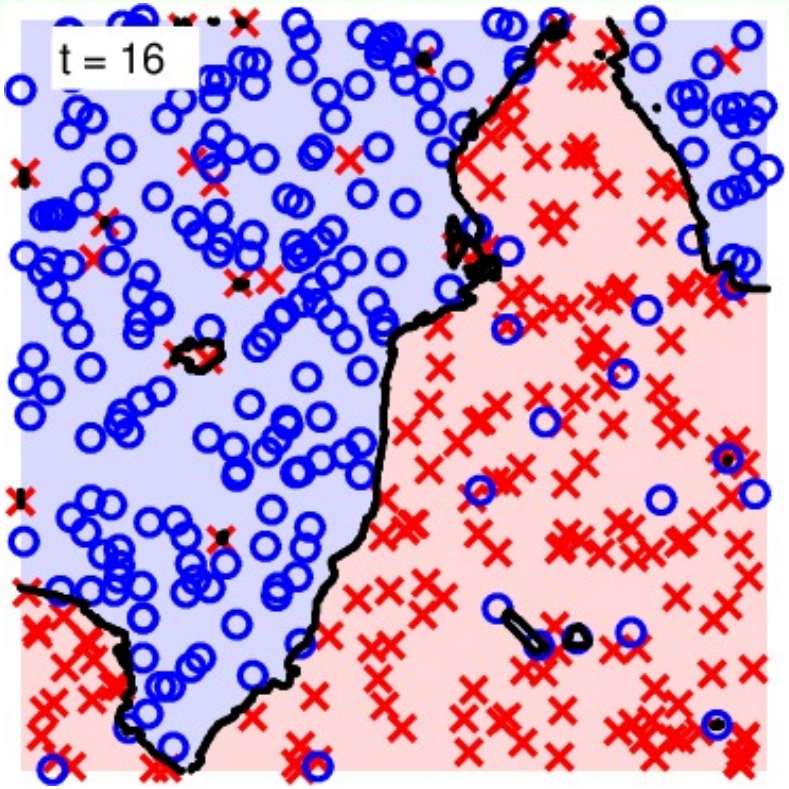

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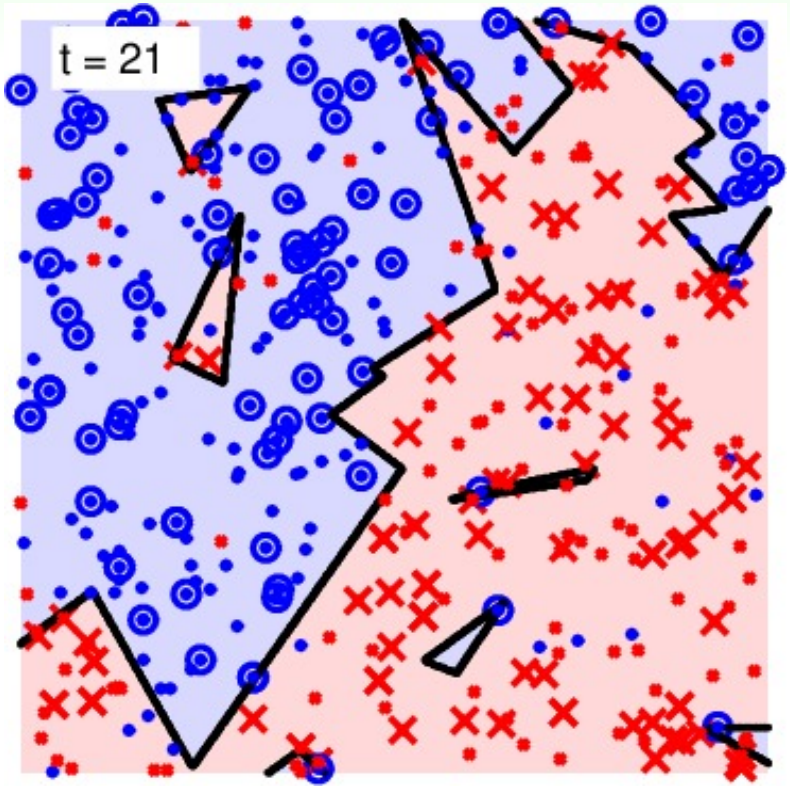

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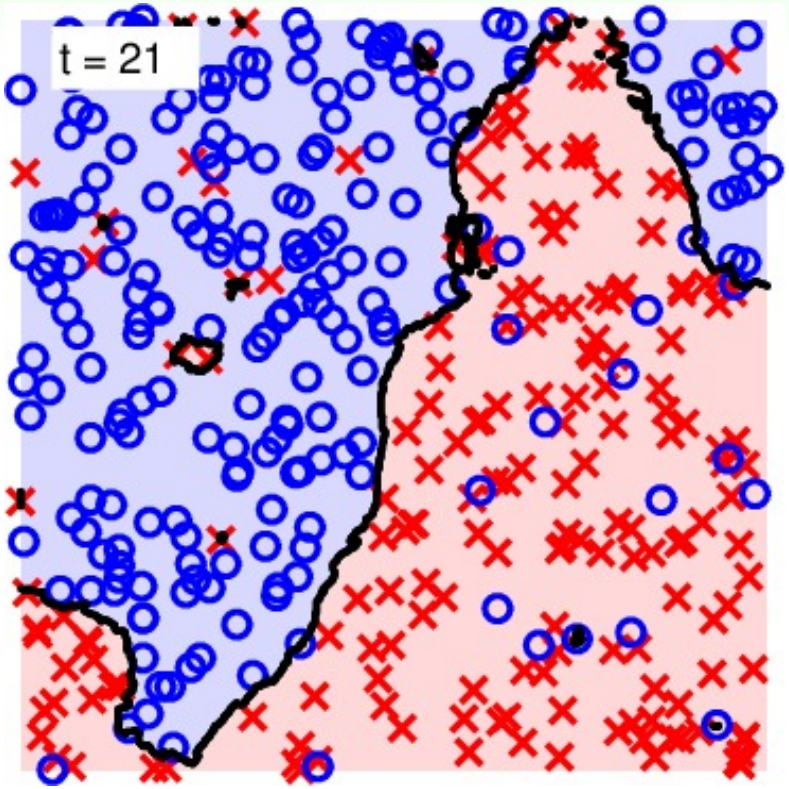

noise corrected by voting

How Many Trees Needed?

almost every theory: the more, **the 'better'**
assuming **good** $\bar{g} = \lim_{T \to \infty} G$

Our NTU Experience

- KDDCup 2013 Track 1 (**yes, NTU is world champion again! :-)**): predicting author-paper relation
- E_{val} of **thousands** of trees: $[0.015, 0.019]$ depending **on seed**; E_{out} of top 20 teams: $[0.014, 0.019]$
- decision: take 12000 **trees** with **seed** 1

cons of RF: may need lots of trees **if the whole random process too unstable**
—should double-check **stability of** G
to ensure **enough trees**

Questions?

AdaBoost Revisited: Example Weights

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

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

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

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

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

- $\text{err}_{0/1}(s, y) = [\![ys \leq 0]\!]$
- $\widehat{\text{err}}_{\text{ADA}}(s, y) = \exp(-ys)$: 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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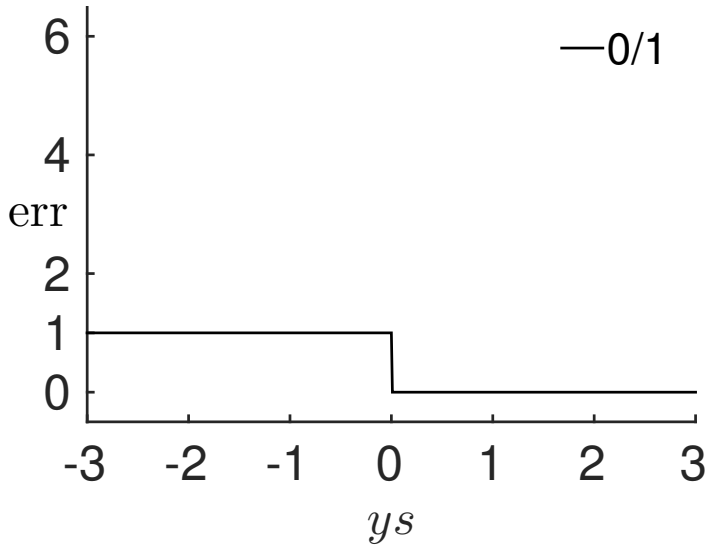

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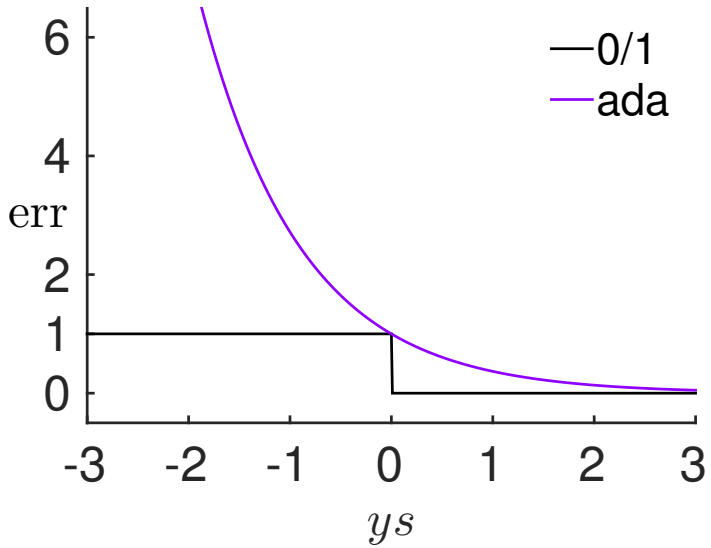


$\widehat{\text{err}}_{\text{ADA}}$: **algorithmic error measure** by **convex upper bound** of $\text{err}_{0/1}$

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

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

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

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

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

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

—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

Questions?

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

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

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

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

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

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

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

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

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 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 + Decision Tree
—**popular in practice**

Questions?

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

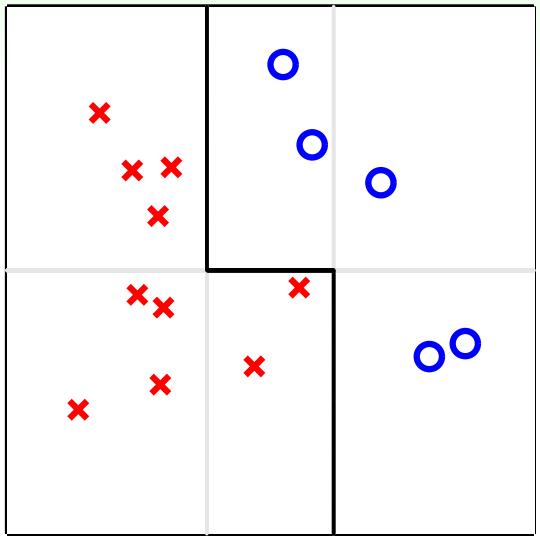
GradientBoost

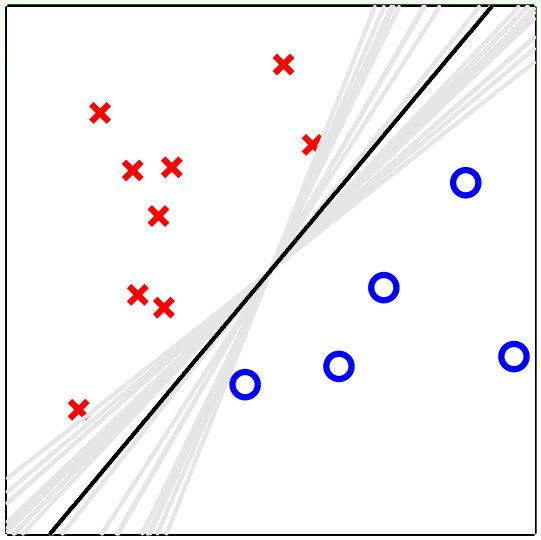
GBDT

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**

Questions?

Summary

1. Combining Predictive Features: Aggregation Models

Lecture 13: Decision Tree Ensembles

- Decision Tree Hypothesis
  express path-conditional aggregation
- Decision Tree Algorithm
  recursive branching until termination to base
- Decision Tree in Action
  explainable and efficient
- Random Forest Algorithm
  bag of trees on randomly projected subspaces
- Out-Of-Bag Estimate
  self-validation with OOB examples
- Random Forest in Action
  'smooth' boundary with many 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