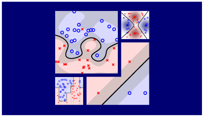
Machine Learning Techniques
(機器學習技法)



Lecture 10: Random Forest

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Roadmap

1. Embedding Numerous Features: Kernel Models
2. Combining Predictive Features: Aggregation Models

Lecture 9: Decision Tree

recursive branching (purification) for **conditional aggregation** of **constant hypotheses**

Lecture 10: Random Forest

- Random Forest Algorithm
- Out-Of-Bag Estimate
- Random Forest in Action

3. Distilling Implicit Features: Extraction Models

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 $G_c \leftarrow$ 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

Fun Time

Within RF that contains random-combination C&RT trees, which of the following hypothesis is equivalent to each branching function $b(\mathbf{x})$ within the tree?

1. a constant
2. a decision stump
3. a perceptron
4. none of the other choices

Fun Time

Within RF that contains random-combination C&RT trees, which of the following hypothesis is equivalent to each branching function $b(\mathbf{x})$ within the tree?

1. a constant
2. a decision stump
3. a perceptron
4. none of the other choices

Reference Answer: ③

In each $b(\mathbf{x})$, the input vector $\mathbf{x}$ is first projected by a random vector $\mathbf{v}$ and then thresholded to make a binary decision, which is exactly what a perceptron does.

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^-
$\mathcal{D}_{\text{train}}$	$\mathcal{D}_{\text{train}}$		$\mathcal{D}_{\text{train}}$
$\mathcal{D}_{\text{val}}$	$\mathcal{D}_{\text{val}}$		$\mathcal{D}_{\text{val}}$
$\mathcal{D}_{\text{val}}$	$\mathcal{D}_{\text{val}}$		$\mathcal{D}_{\text{val}}$
$\mathcal{D}_{\text{train}}$	$\mathcal{D}_{\text{train}}$		$\mathcal{D}_{\text{train}}$

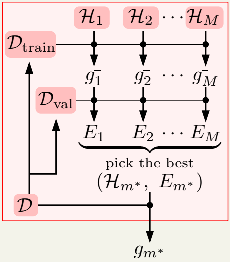
- $\star$ like $\mathcal{D}_{\text{val}}$: 'enough' random examples unused during training
- use $\star$ to validate g_t? easy, but **rarely needed**
- use $\star$ to validate G? $E_{\text{oob}}(G) = \frac{1}{N}\sum_{n=1}^{N} \text{err}(y_n, G_n^-(\mathbf{x}_n))$, with G_n^- contains only trees that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

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



RF: by Best E_{oob}

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

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

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

Fun Time

For a data set with $N = 1126$, what is the probability that $(\mathbf{x}_{1126}, y_{1126})$ is not sampled after bootstrapping $N' = N$ samples from the data set?

1. 0.113
2. 0.368
3. 0.632
4. 0.887

Fun Time

For a data set with $N = 1126$, what is the probability that $(\mathbf{x}_{1126}, y_{1126})$ is not sampled after bootstrapping $N' = N$ samples from the data set?

1. 0.113
2. 0.368
3. 0.632
4. 0.887

Reference Answer: ②

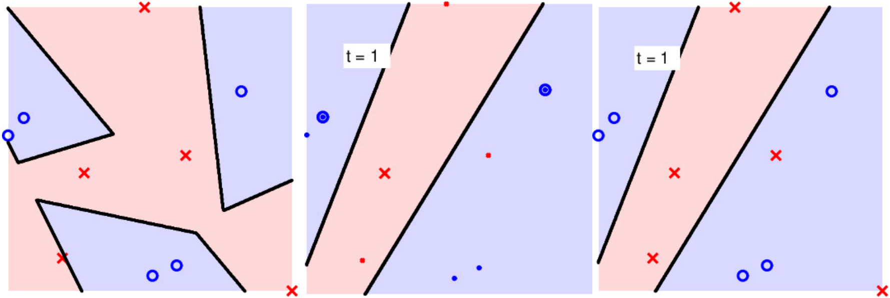
The value of $(1 - \frac{1}{N})^N$ with $N = 1126$ is about 0.367716, which is close to $\frac{1}{e} = 0.367879$.

A Simple Data Set

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

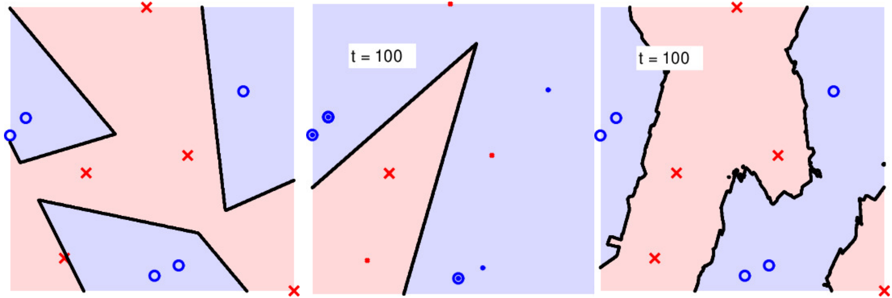
g_t $(N' = N/2)$

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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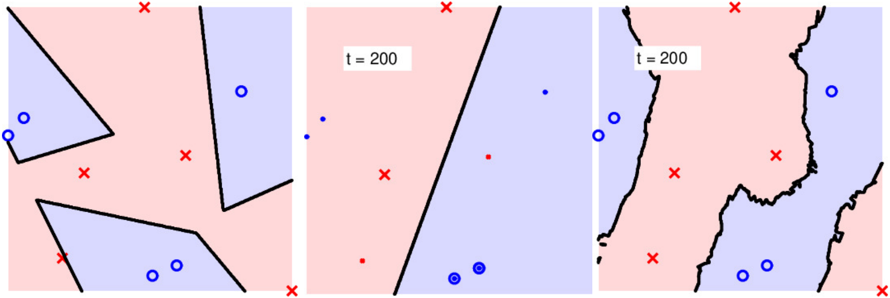

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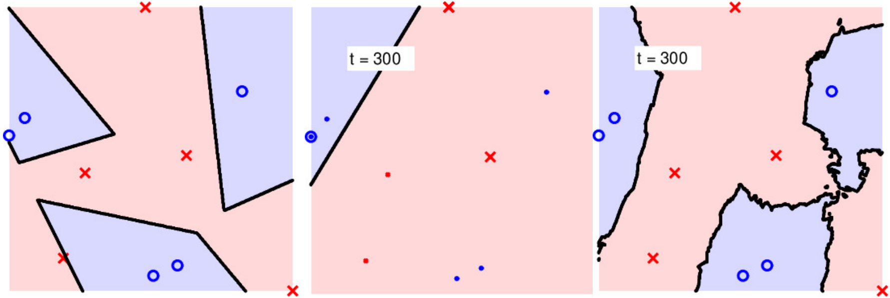

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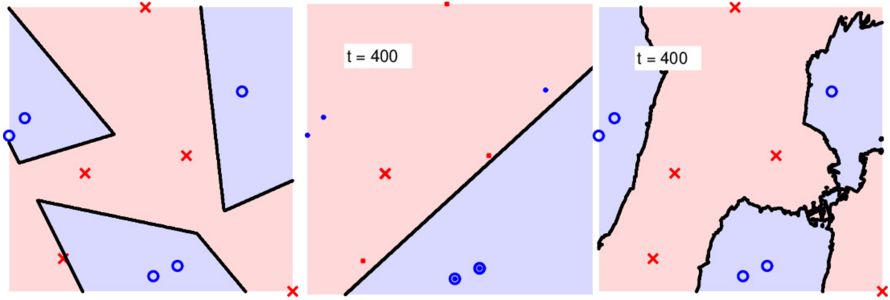

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$g_{\text{C\&RT}}$ with random combination

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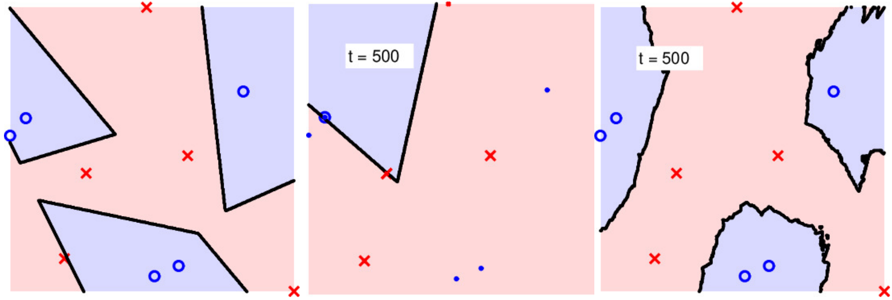

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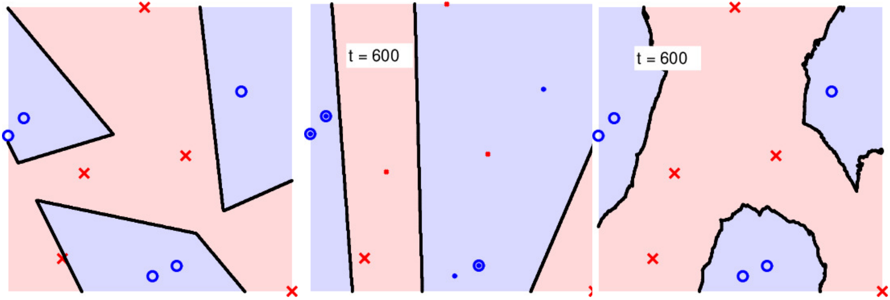

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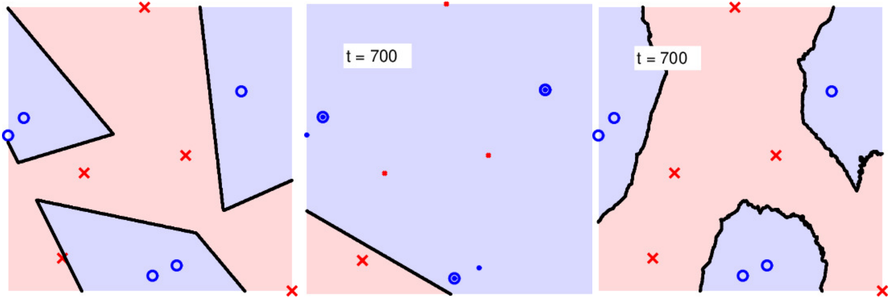

A Simple Data Set

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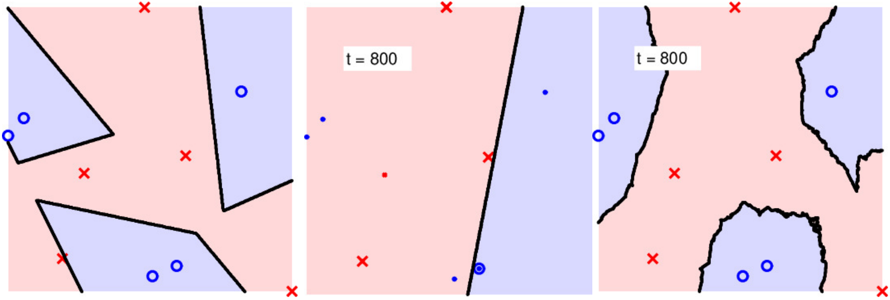

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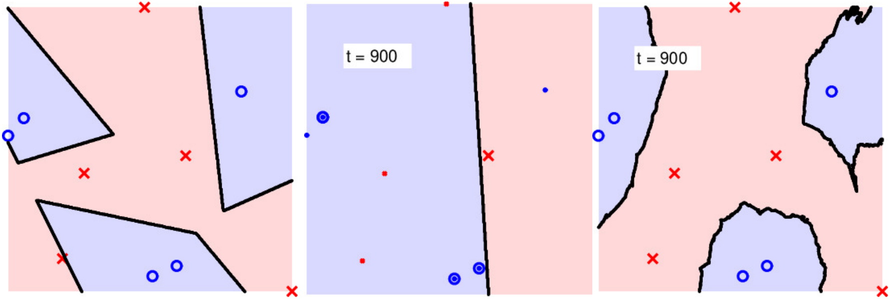
$g_{\text{C\&RT}}$ with random combination	g_t $(N' = N/2)$	G with first t trees



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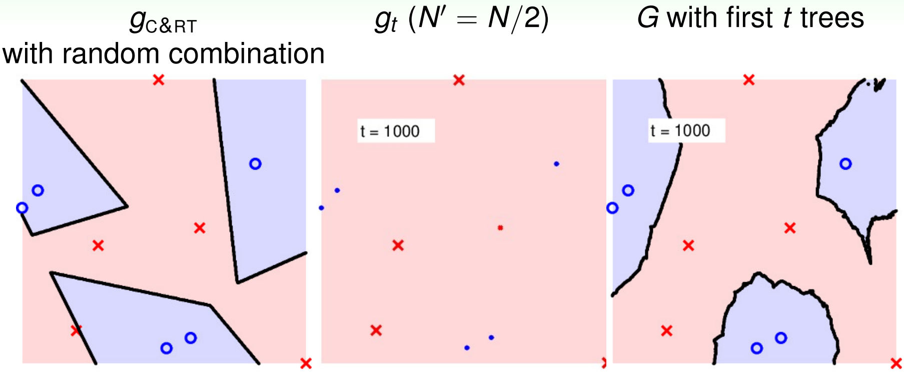
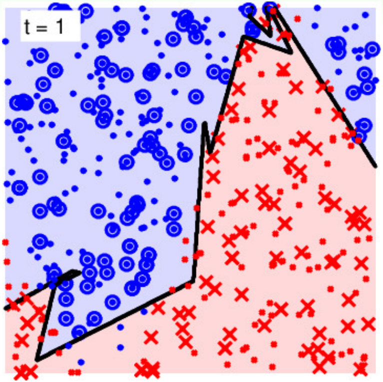


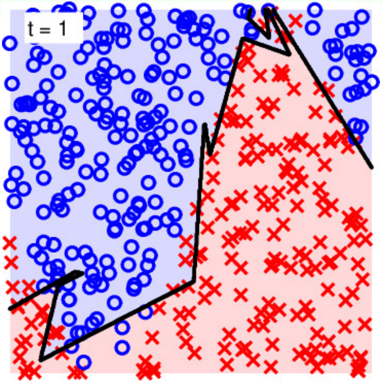
'smooth' and large-margin-like boundary with many trees

A Complicated Data Set

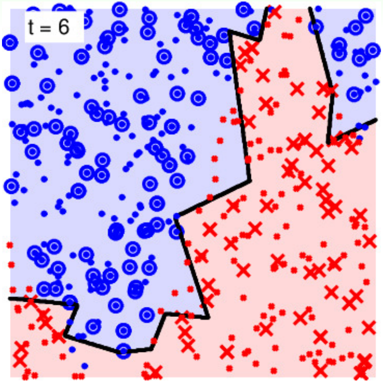
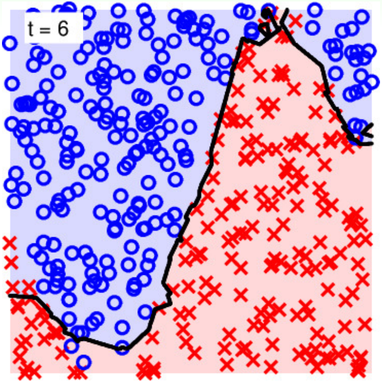
g_t $(N' = N/2)$



G with first t trees



A Complicated Data Set

g_t ($N' = N/2$)	G with first t trees
	

A Complicated Data Set

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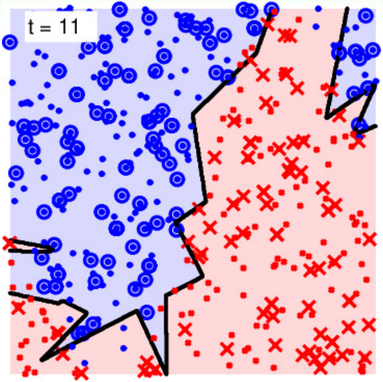

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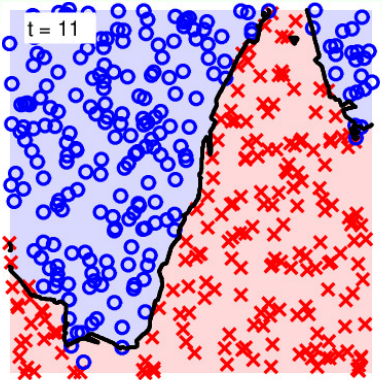
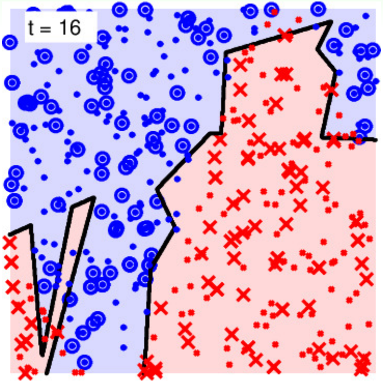
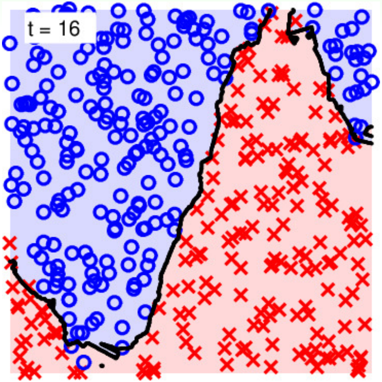


A Complicated Data Set

g_t $(N' = N/2)$

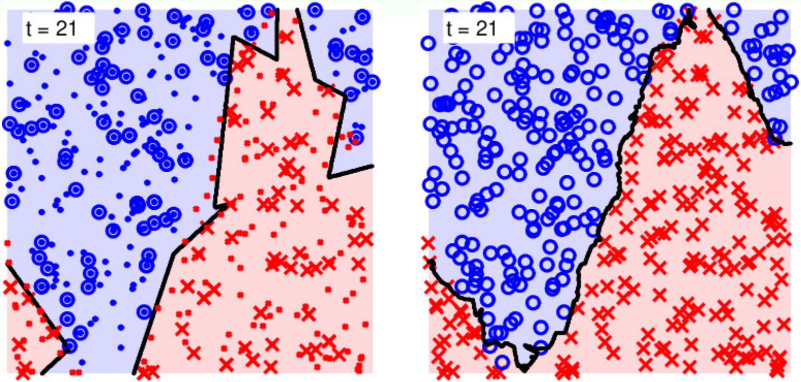


G with first t trees



A Complicated Data Set

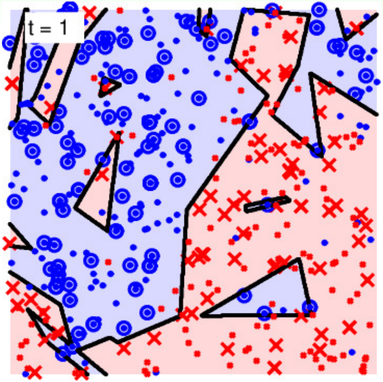
g_t $(N' = N/2)$ — G with first t trees



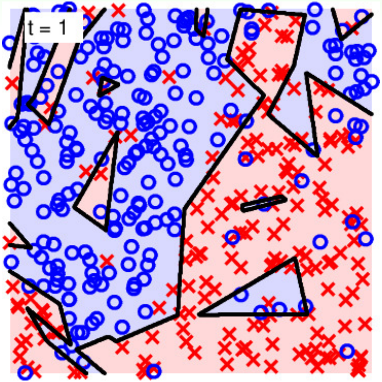
'easy yet robust' nonlinear model

A Complicated and Noisy Data Set

g_t $(N' = N/2)$

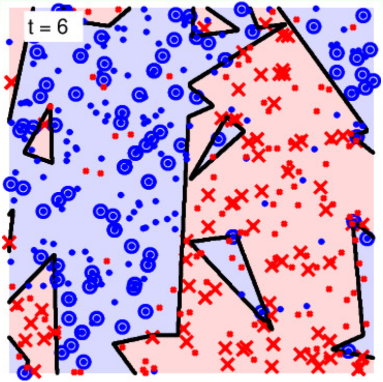


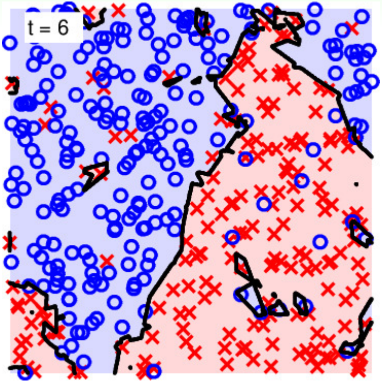
G with first t trees



A Complicated and Noisy Data Set

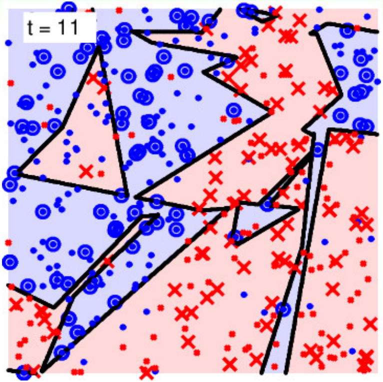
g_t $(N' = N/2)$ | G with first t trees



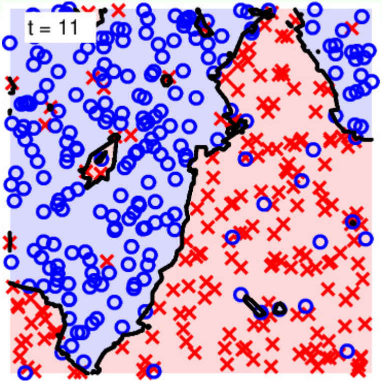


A Complicated and Noisy Data Set

g_t $(N' = N/2)$

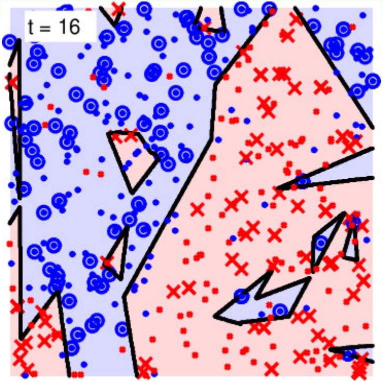


G with first t trees

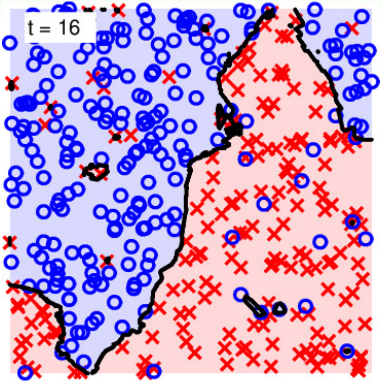


A Complicated and Noisy Data Set

g_t ($N' = N/2$)

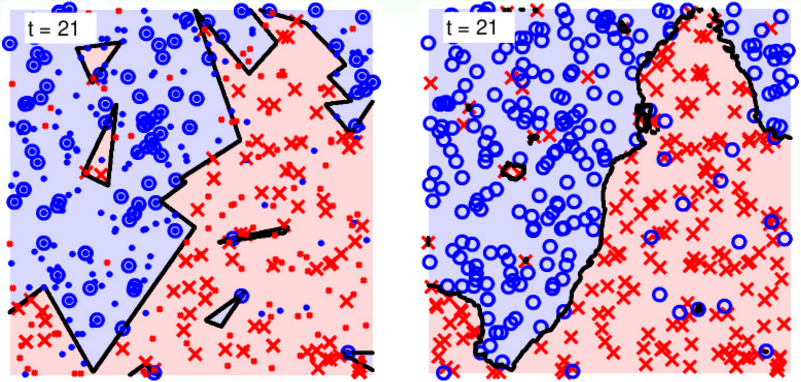


G with first t trees



A Complicated and Noisy Data Set

g_t $(N' = N/2)$ · G with first t trees



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**

Fun Time

Which of the following is **not** the best use of Random Forest?

1. train each tree with bootstrapped data
2. use E_{oob} to validate the performance
3. conduct feature selection with permutation test
4. fix the number of trees, T, to the lucky number 1126

Fun Time

Which of the following is **not** the best use of Random Forest?

1. train each tree with bootstrapped data
2. use E_{oob} to validate the performance
3. conduct feature selection with permutation test
4. fix the number of trees, T, to the lucky number 1126

Reference Answer: ④

A good value of T can depend on the nature of the data and the stability of the whole random process.

Summary

1. Embedding Numerous Features: Kernel Models
2. Combining Predictive Features: Aggregation Models

Lecture 10: Random Forest

- 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

- **next: boosted decision trees beyond classification**

3. Distilling Implicit Features: Extraction Models