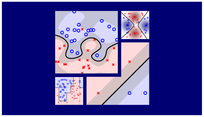
Machine Learning Techniques
(機器學習技法)



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
- Feature Selection
- 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 $G_c \leftarrow \text{DTree}(\mathcal{D}_c)$
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 Projection

recall: **data randomness** for **diversity** in **bagging**

randomly **sample N' examples** from $\mathcal{D}$

another possibility for **diversity**:

randomly **sample d' features** from $\mathbf{x}$

- when sampling index $i_1, i_2, \ldots, i_{d'}$: $\mathbf{\Phi}(\mathbf{x}) = (x_{i_1}, x_{i_2}, \ldots, x_{i_{d'}})$
- $\mathcal{Z} \in \mathbb{R}^{d'}$: a **random subspace** of $\mathcal{X} \in \mathbb{R}^{d}$
- often $d' \ll d$, efficient for large d
  —can be generally applied on other models
- original RF **re-sample new subspace for each $b(\mathbf{x})$ in C&RT**

RF = bagging + random-subspace C&RT

Diversifying by Feature Expansion

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

more **powerful** features for **diversity**: row i other than natural basis

- **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 $\mathbf{p}_i$
- includes **random subspace** as **special case**:
  $d'' = 1$ and $\mathbf{p}_i \in$ natural basis
- original RF consider d' random **low-dimensional projections for each** $b(\mathbf{x})$ in C&RT

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

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

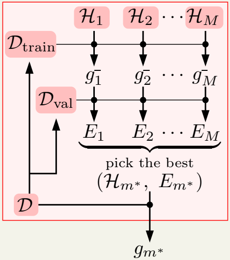
- $\star$ like $\mathcal{D}_{\text{val}}$: 'enough' random examples unused during training
- use $\star$ to validate g_t? easy, but **rarely needed**
- use $\star$ to validate G? $E_{\text{oob}}(G) = \frac{1}{N}\sum_{n=1}^{N} \text{err}(y_n, G_n^-(\mathbf{x}_n))$, with G_n^- contains only trees that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

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



RF: by Best E_{oob}

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

- 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 $\frac{1}{e} = 0.367879$.

Feature Selection

for $\mathbf{x} = (x_1, x_2, \ldots, x_d)$, want to remove

- **redundant** features: like keeping one of 'age' and 'full birthday'
- **irrelevant** features: like insurance type for cancer prediction

and only 'learn' **subset-transform** $\mathbf{\Phi}(\mathbf{x}) = (x_{i_1}, x_{i_2}, x_{i_{d'}})$ with $d' < d$ for $g(\mathbf{\Phi}(\mathbf{x}))$

advantages:

- **efficiency**: simpler hypothesis and shorter prediction time
- **generalization**: 'feature noise' removed
- **interpretability**

disadvantages:

- **computation**: 'combinatorial' optimization in training
- **overfit**: 'combinatorial' selection
- **mis-interpretability**

decision tree: a rare model with **built-in feature selection**

Feature Selection by Importance

idea: if possible to calculate

$$\text{importance}(i) \text{ for } i = 1, 2, \ldots, d$$

then can select $i_1, i_2, \ldots, i_{d'}$ of top-d' importance

importance by linear model

$$\text{score} = \mathbf{w}^T\mathbf{x} = \sum_{i=1}^{d} w_i x_i$$

- intuitive estimate: $\text{importance}(i) = |w_i|$ with some 'good' $\mathbf{w}$
- getting 'good' $\mathbf{w}$: learned from data
- non-linear models? often **much harder**

next: **'easy'** feature selection in RF

Feature Importance by Permutation Test

idea: random test
—if feature i needed, 'random' values of $x_{n,i}$ degrades performance

- which random values?
  - uniform, Gaussian, ...: $P(x_i)$ changed
  - bootstrap, **permutation** (of $\{x_{n,i}\}_{n=1}^{N}$): $P(x_i)$ approximately remained
- **permutation** test:

$$\text{importance}(i) = \text{performance}(\mathcal{D}) - \text{performance}(\mathcal{D}^{(p)})$$

with $\mathcal{D}^{(p)}$ is $\mathcal{D}$ with $\{x_{n,i}\}$ replaced by permuted $\{x_{n,i}\}_{n=1}^{N}$

permutation test: a general statistical tool for arbitrary non-linear models like RF

Feature Importance in Original Random Forest

permutation test:

$$\text{importance}(i) = \text{performance}(\mathcal{D}) - \text{performance}(\mathcal{D}^{(p)})$$

with $\mathcal{D}^{(p)}$ is $\mathcal{D}$ with $\{x_{n,i}\}$ replaced by permuted $\{x_{n,i}\}_{n=1}^{N}$

- performance($\mathcal{D}^{(p)}$): needs re-training and validation in general
- **'escaping' validation**? **OOB** in RF
- original RF solution: importance(i) $= E_{\text{oob}}(G) - E_{\text{oob}}^{(p)}(G)$, where $E_{\text{oob}}^{(p)}$ comes from replacing each request of $x_{n,i}$ by a **permuted OOB** value

RF **feature selection** via **permutation** + **OOB**:
often efficient and promising in practice

Fun Time

For RF, if the 1126-th feature within the data set is a constant 5566, what would importance(i) be?

1. 0
2. 1
3. 1126
4. 5566

Fun Time

For RF, if the 1126-th feature within the data set is a constant 5566, what would importance(i) be?

1. 0
2. 1
3. 1126
4. 5566

Reference Answer: 1

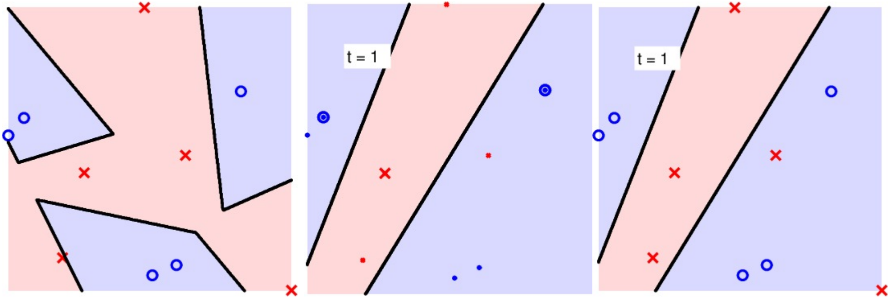
When a feature is a constant, permutation does not change its value. Then, $E_{\text{oob}}(G)$ and $E_{\text{oob}}^{(p)}(G)$ are the same, and thus importance(i) $= 0$.

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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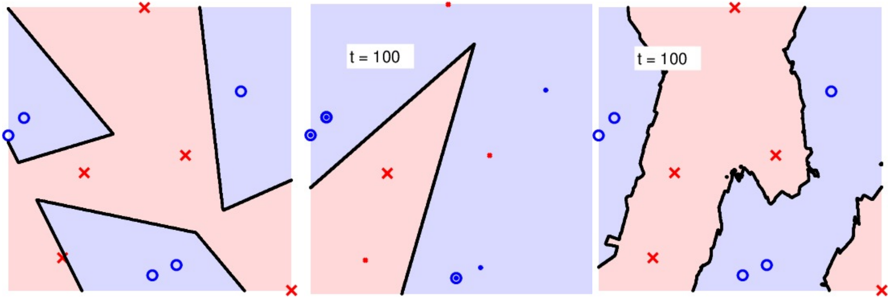

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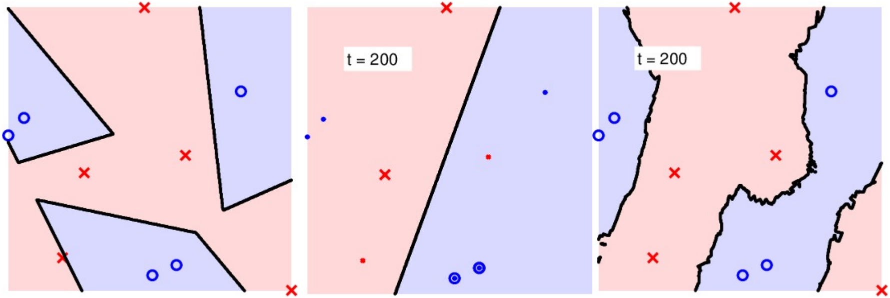

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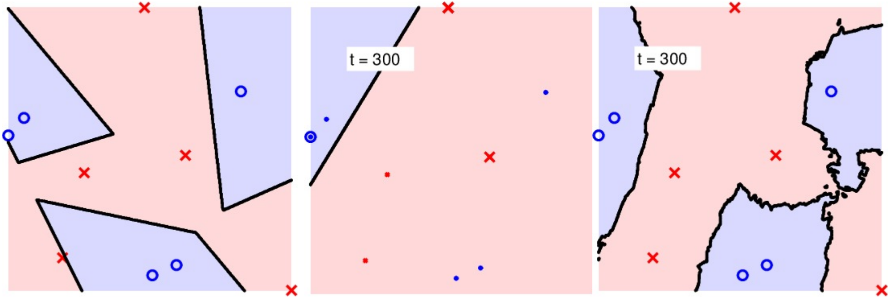

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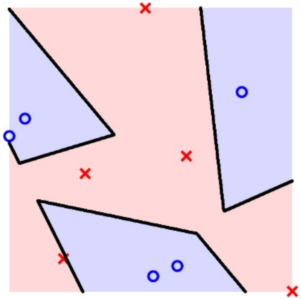
$g_{\text{C\&RT}}$ with random combination



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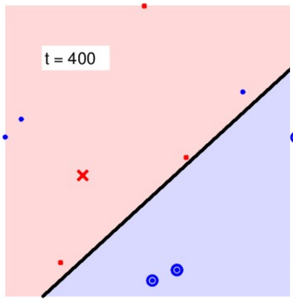
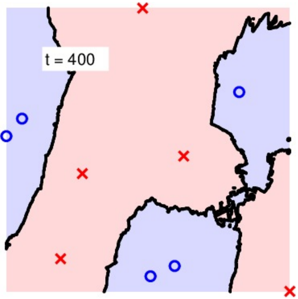


G with first t trees



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

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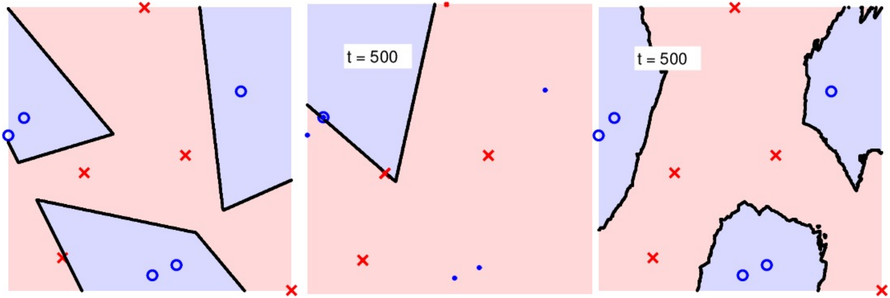

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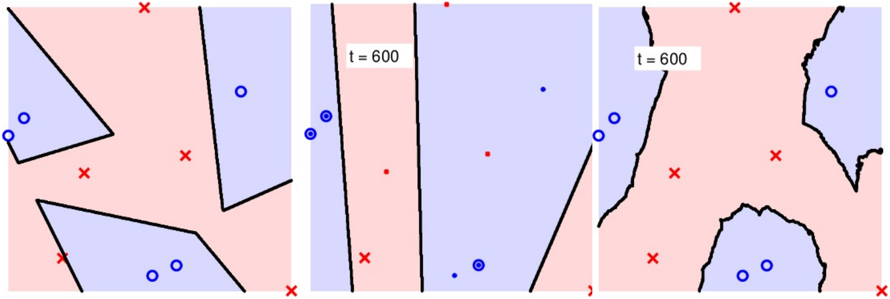

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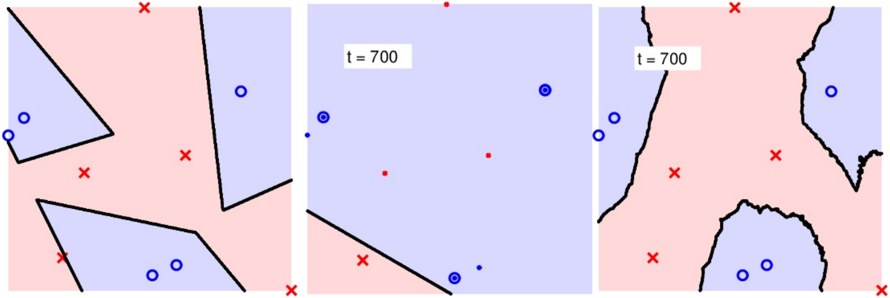

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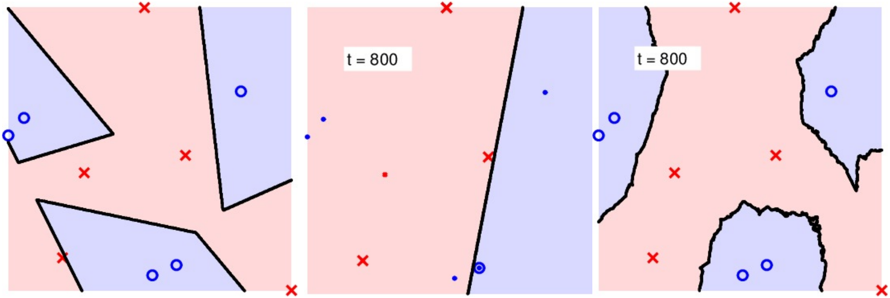

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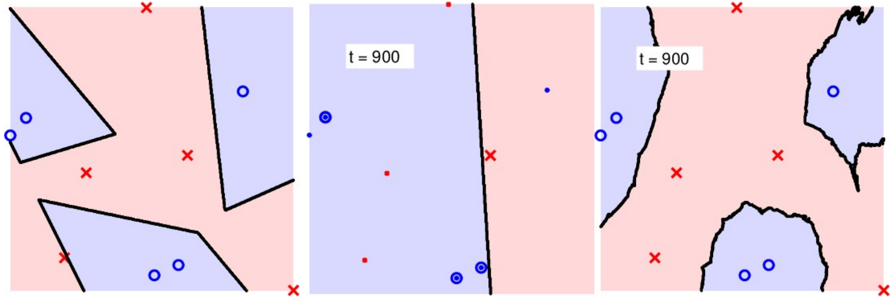
$g_{\text{C\&RT}}$ with random combination | g_t ($N' = N/2$) | G with first t trees



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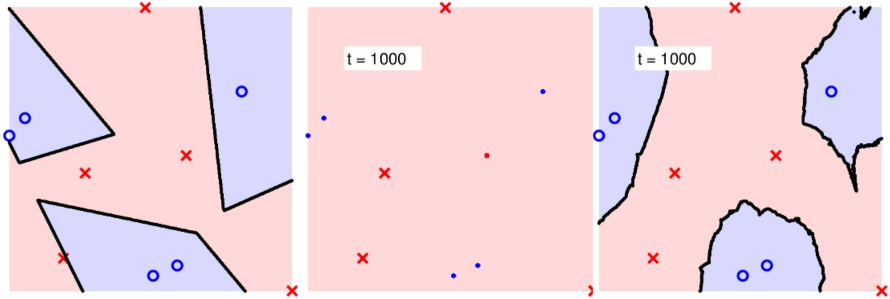
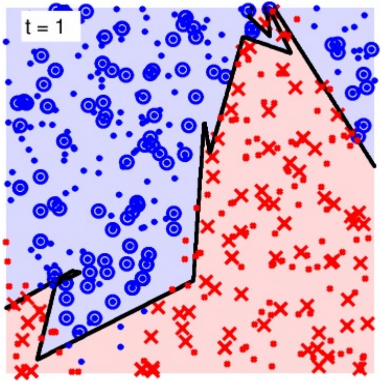
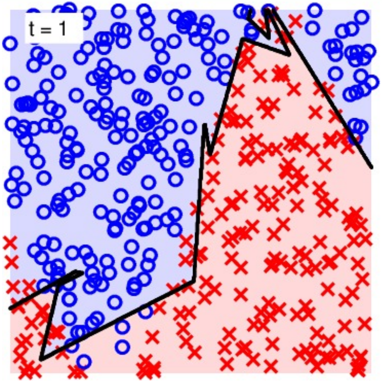


'smooth' and large-margin-like boundary with many trees

A Complicated Data Set

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





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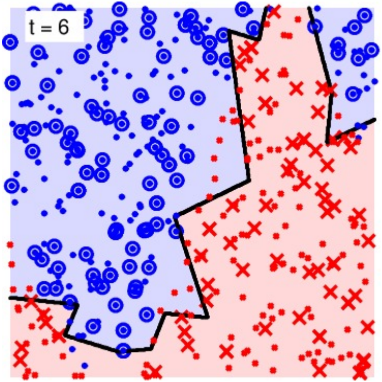
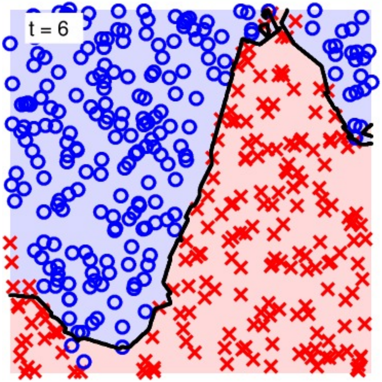
g_t ($N' = N/2$)



G with first t trees



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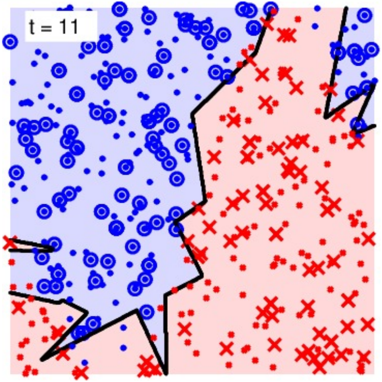
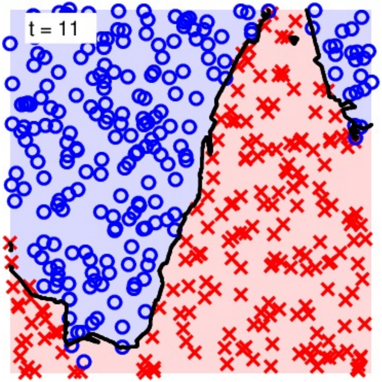
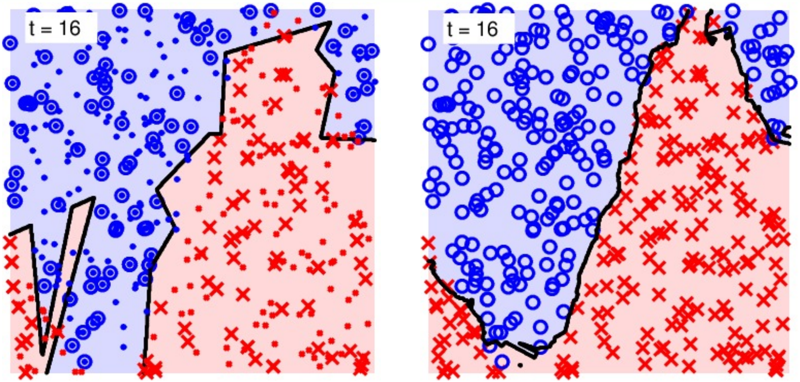


G with first t trees



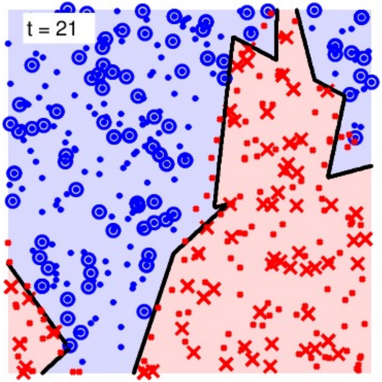
A Complicated Data Set

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

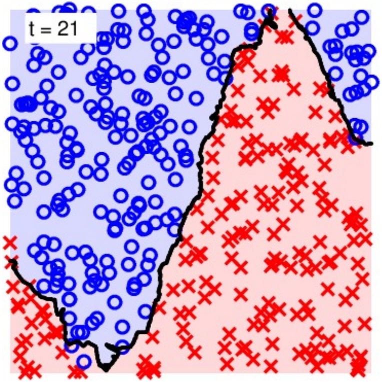


A Complicated Data Set

g_t $(N' = N/2)$



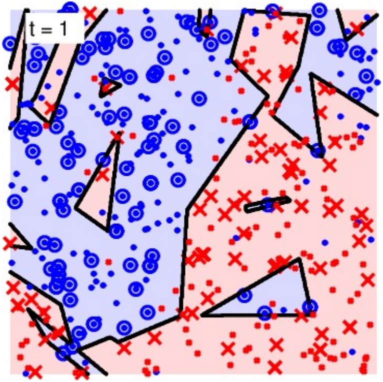
G with first t trees



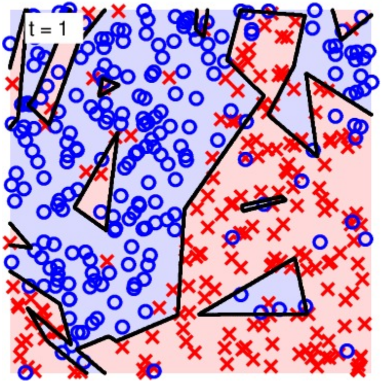
'easy yet robust' nonlinear model

A Complicated and Noisy Data Set

g_t ($N' = N/2$)

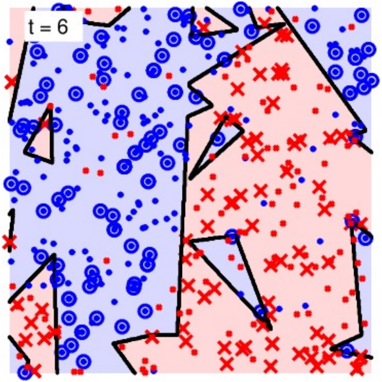


G with first t trees

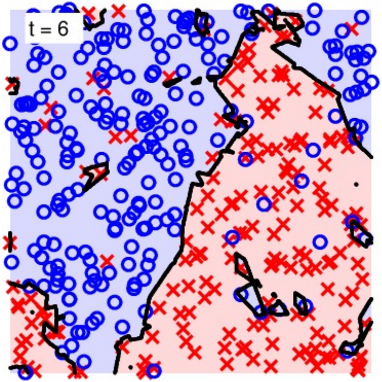


A Complicated and Noisy Data Set

g_t ($N' = N/2$)



G with first t trees



A Complicated and Noisy Data Set

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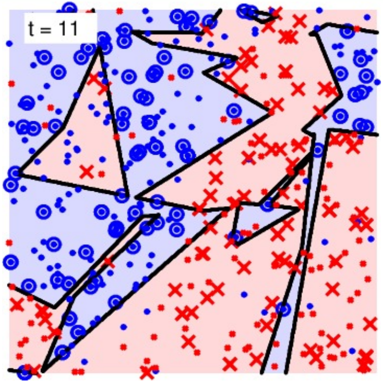
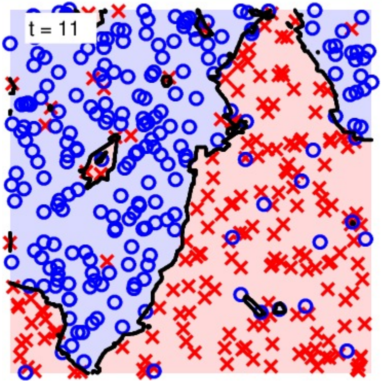


G with first t trees



A Complicated and Noisy Data Set

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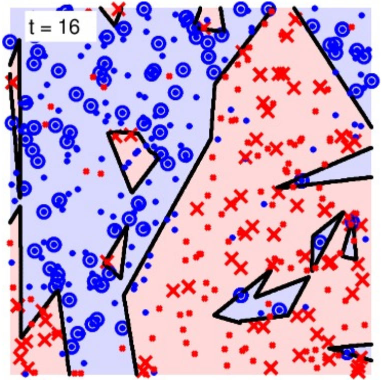
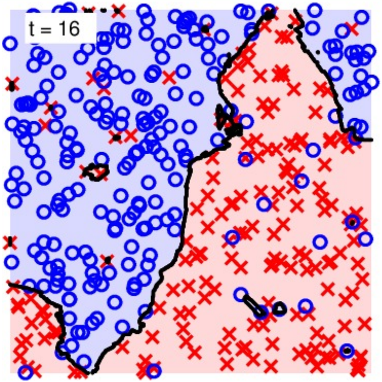


G with first t trees



A Complicated and Noisy Data Set

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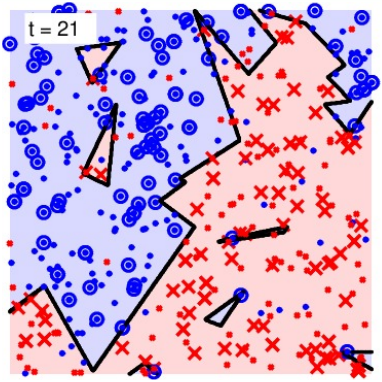
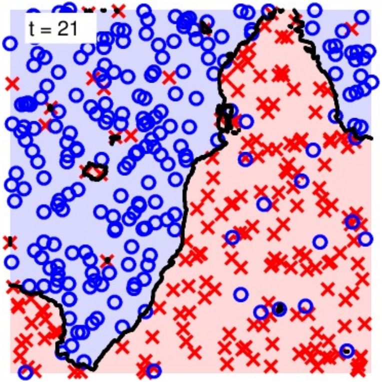


G with first t trees



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
- Feature Selection

  permutation test for feature importance
- Random Forest in Action

  'smooth' boundary with many trees

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

3. Distilling Implicit Features: Extraction Models