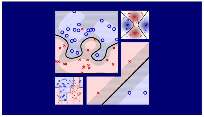
# Machine Learning Techniques
# (機器學習技法)



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

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**(i.e. aggregation of aggregation :-) )**

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- **eliminate cons** of fully-grown tree

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RF = bagging + random-subspace C&RT

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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
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**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.

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

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

# OOB versus Validation

## OOB

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| $(\mathbf{x}_N, y_N)$ | $\tilde{\mathcal{D}}_1$ | $\star$ | $\star$ | | $\star$ |

# OOB versus Validation

## OOB

| | $g_1$ | $g_2$ | $g_3$ | $\cdots$ | $g_T$ |
|---|---|---|---|---|---|
| $(\mathbf{x}_1, y_1)$ | $\tilde{\mathcal{D}}_1$ | $\star$ | $\tilde{\mathcal{D}}_3$ | | $\tilde{\mathcal{D}}_T$ |
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| $(\mathbf{x}_3, y_3)$ | $\star$ | $\tilde{\mathcal{D}}_2$ | $\star$ | | $\tilde{\mathcal{D}}_T$ |
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## Validation

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

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## Validation

| $g_1^-$ | $g_2^-$ | $\cdots$ | $g_M^-$ |
|---|---|---|---|
| $\mathcal{D}_{\text{train}}$ | $\mathcal{D}_{\text{train}}$ | | $\mathcal{D}_{\text{train}}$ |
| $\mathcal{D}_{\text{val}}$ | $\mathcal{D}_{\text{val}}$ | | $\mathcal{D}_{\text{val}}$ |
| $\mathcal{D}_{\text{val}}$ | $\mathcal{D}_{\text{val}}$ | | $\mathcal{D}_{\text{val}}$ |
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|---|---|---|---|
| $\mathcal{D}_{\text{train}}$ | $\mathcal{D}_{\text{train}}$ | | $\mathcal{D}_{\text{train}}$ |
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| $\mathcal{D}_{\text{train}}$ | $\mathcal{D}_{\text{train}}$ | | $\mathcal{D}_{\text{train}}$ |
| $\mathcal{D}_{\text{val}}$ | $\mathcal{D}_{\text{val}}$ | | $\mathcal{D}_{\text{val}}$ |
| $\mathcal{D}_{\text{val}}$ | $\mathcal{D}_{\text{val}}$ | | $\mathcal{D}_{\text{val}}$ |
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| $\mathcal{D}_{\text{val}}$ | $\mathcal{D}_{\text{val}}$ | | $\mathcal{D}_{\text{val}}$ |
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|---|---|---|---|
| $\mathcal{D}_{\text{train}}$ | $\mathcal{D}_{\text{train}}$ | | $\mathcal{D}_{\text{train}}$ |
| $\mathcal{D}_{\text{val}}$ | $\mathcal{D}_{\text{val}}$ | | $\mathcal{D}_{\text{val}}$ |
| $\mathcal{D}_{\text{val}}$ | $\mathcal{D}_{\text{val}}$ | | $\mathcal{D}_{\text{val}}$ |
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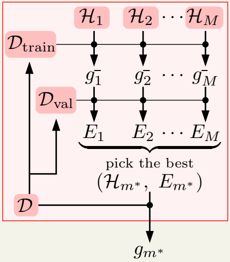
$E_{\text{oob}}$: self-validation of bagging/RF

# Model Selection by OOB Error

## Previously: by Best $E_{\text{val}}$

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



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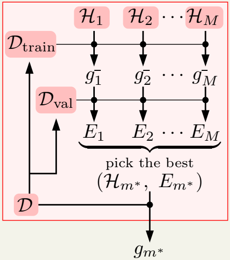


## RF: by Best $E_{\text{oob}}$

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

- use $E_{\text{oob}}$ for self-validation

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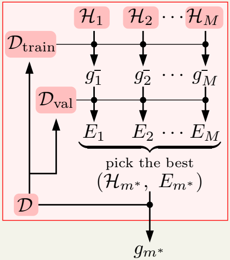


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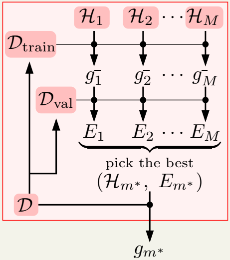


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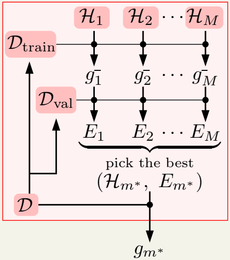


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$E_{\text{oob}}$ often **accurate** in practice

# 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

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

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

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

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

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

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

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

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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
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**Reference Answer: 1**

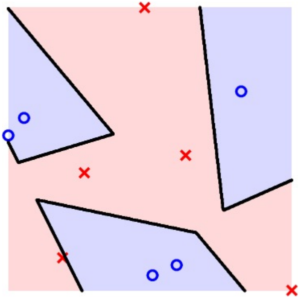
When a feature is a constant, permutation does not change its value. Then, $E_{\text{oob}}(G)$ and $E^{(p)}_{\text{oob}}(G)$ are the same, and thus importance($i$) $= 0$.

# 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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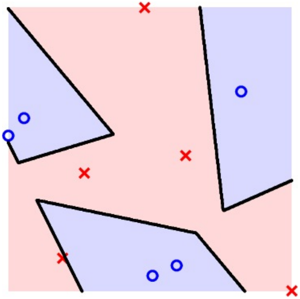

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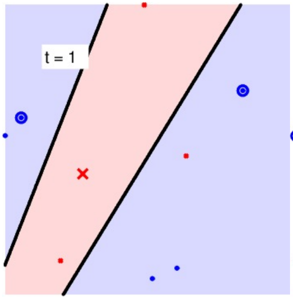


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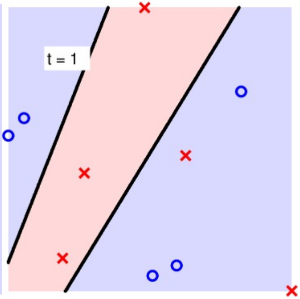

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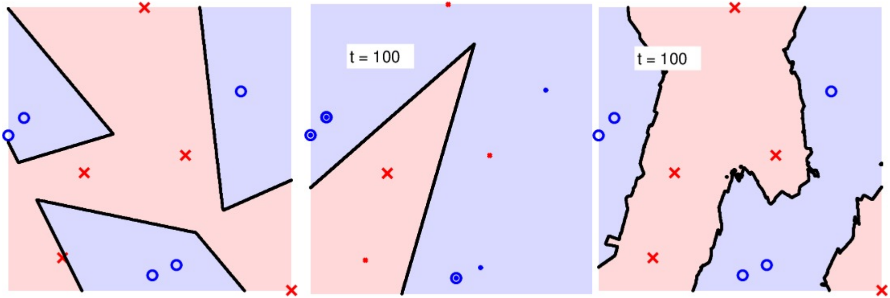

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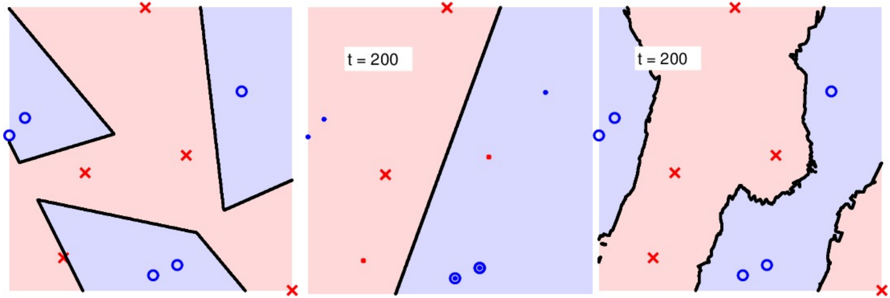

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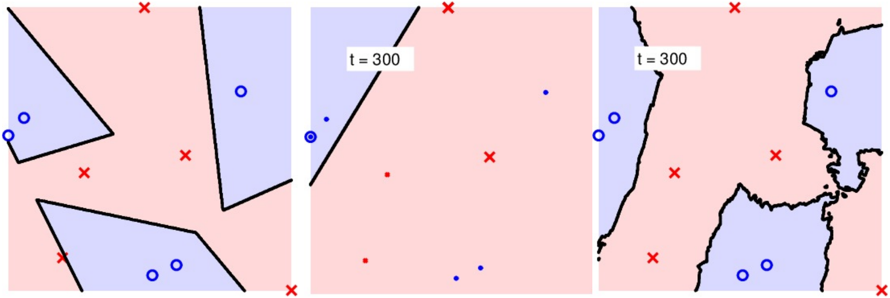

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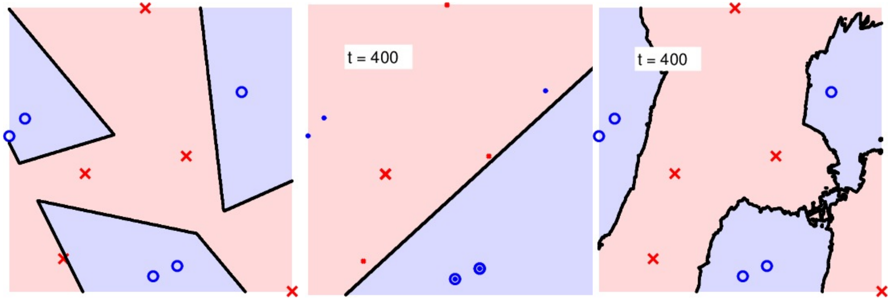

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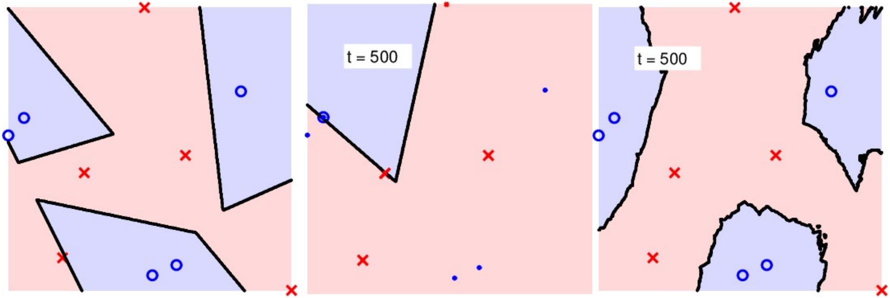

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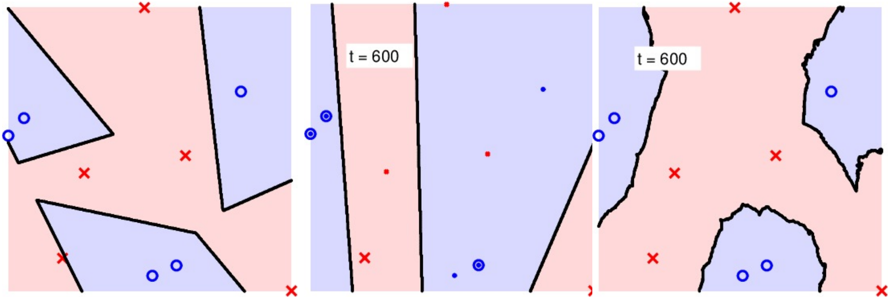

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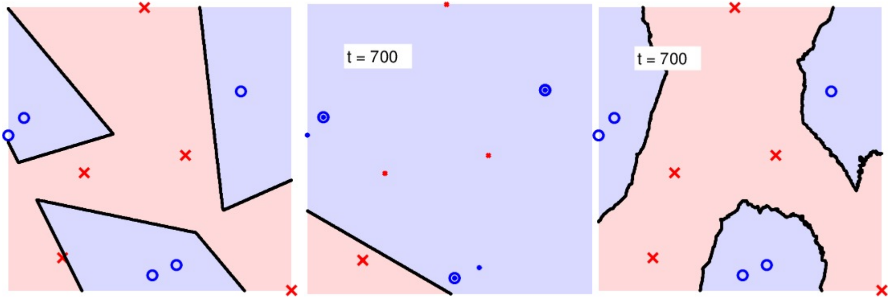

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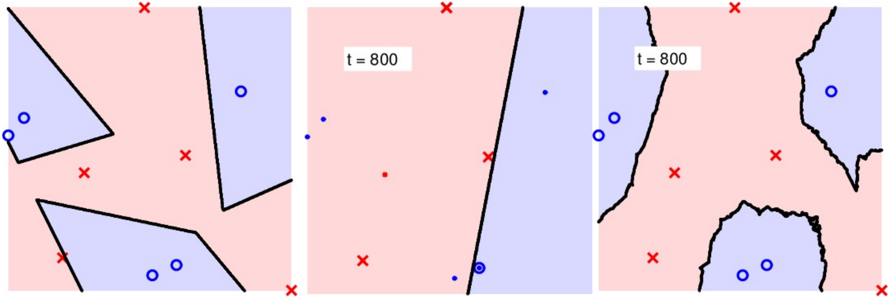

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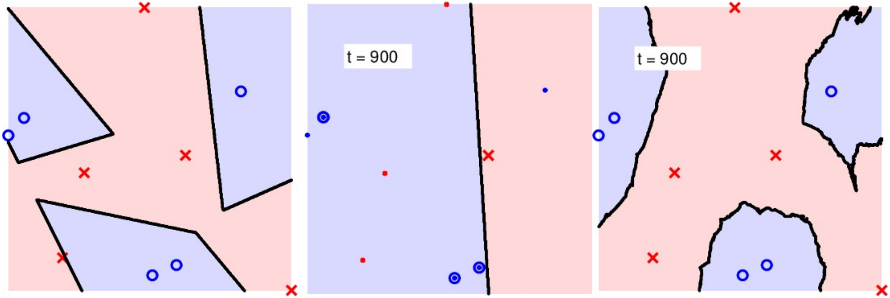

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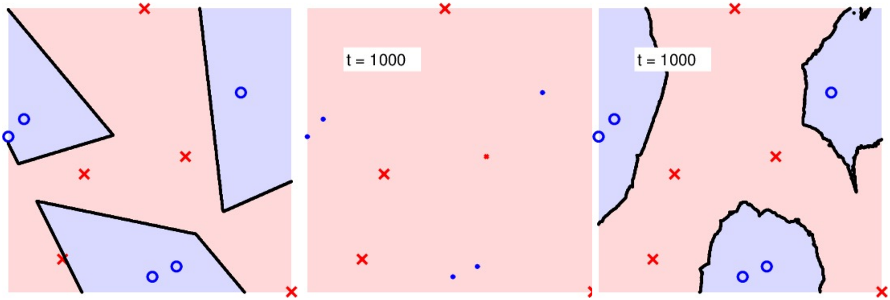


**'smooth' and large-margin-like boundary with many trees**

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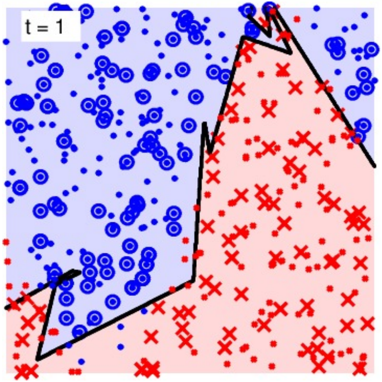


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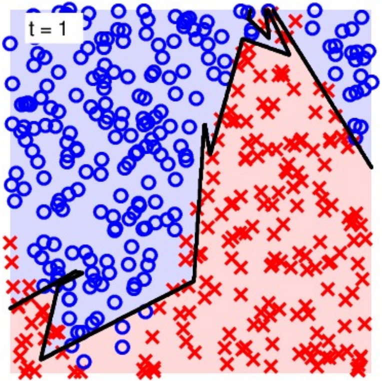

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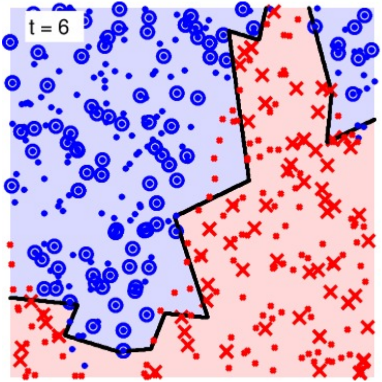


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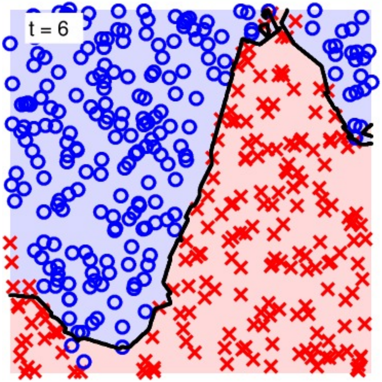

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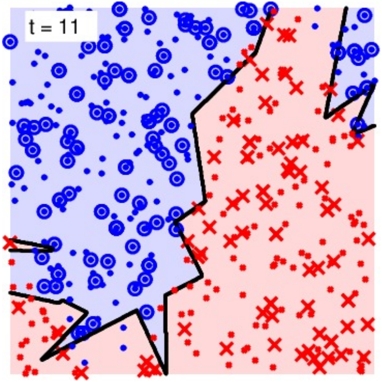

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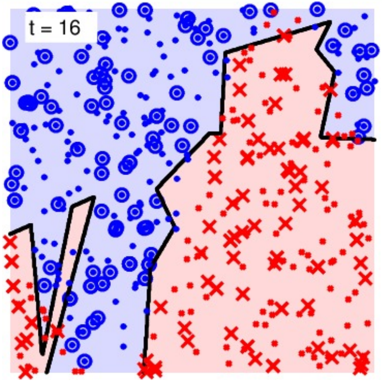


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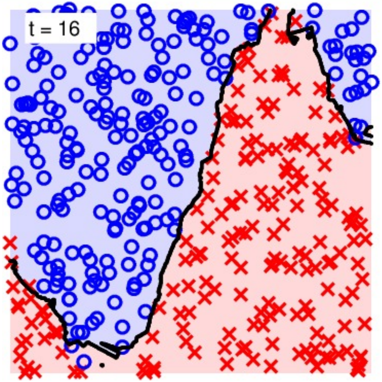

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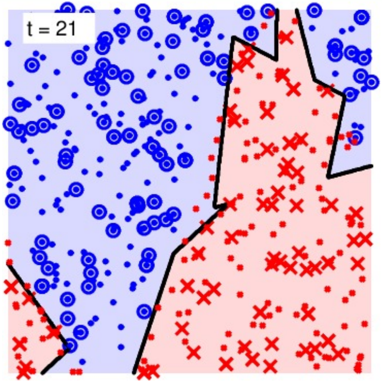


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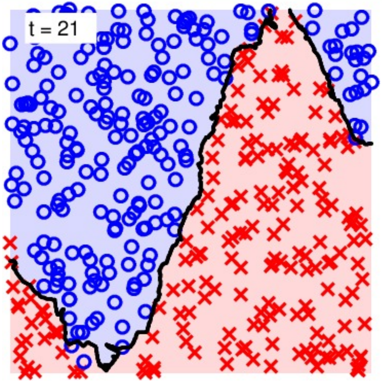


**'easy yet robust' nonlinear model**

# A Complicated and Noisy Data Set

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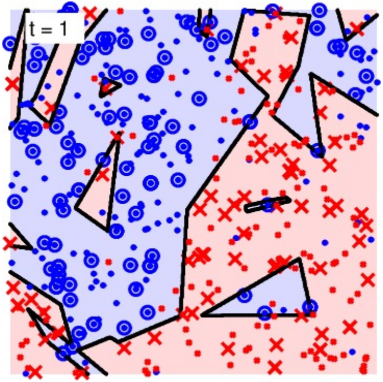


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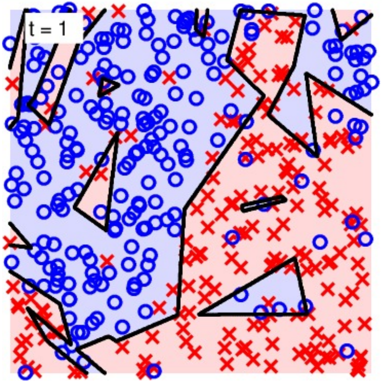

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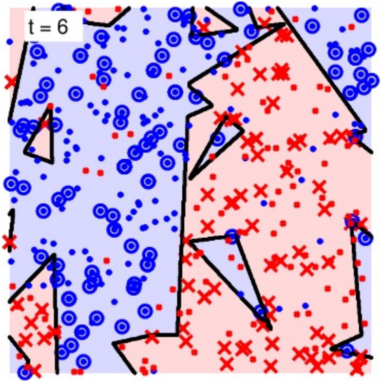


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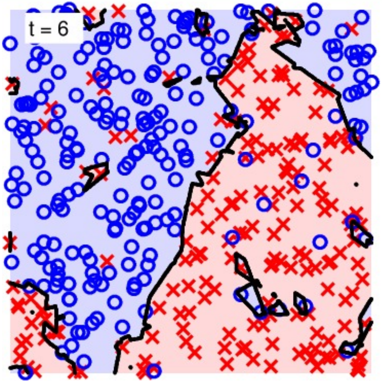

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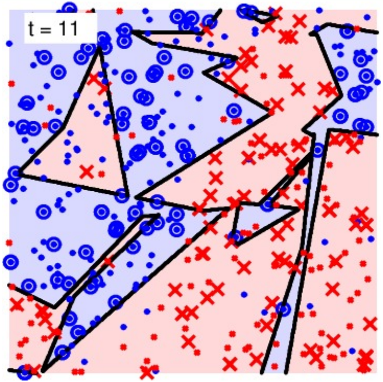


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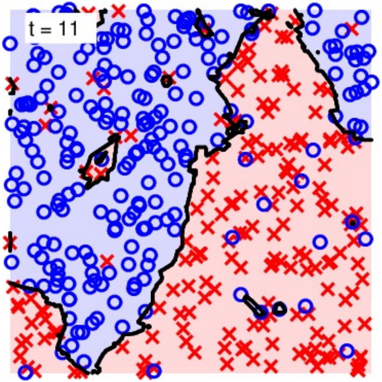

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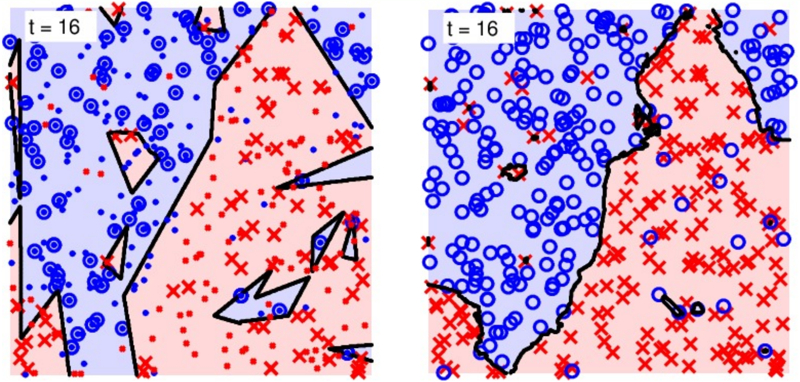

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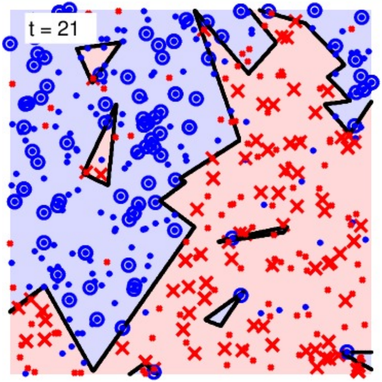


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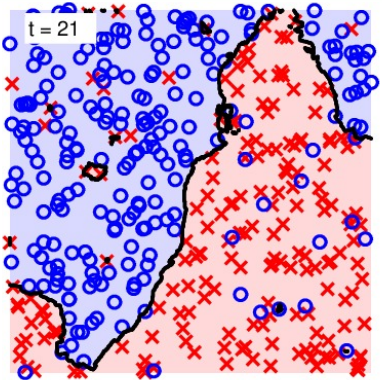


**noise corrected** by voting

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cons of RF: may need lots of trees **if the whole random process too unstable**

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- $E_{\text{val}}$ of **thousands** of trees: $[0.015, 0.019]$ depending **on seed**; $E_{\text{out}}$ 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 $E_{\text{oob}}$ 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