

Ensemble

Framework of Ensemble

團隊合作: 好幾個模型一起上
通常可讓performance提升一個level

- Get a set of classifiers

- $f_1(x), f_2(x), f_3(x), \dots$

↓ ↓ ↓
坦 補 DD

希望每個classifiers有不同屬性/作用

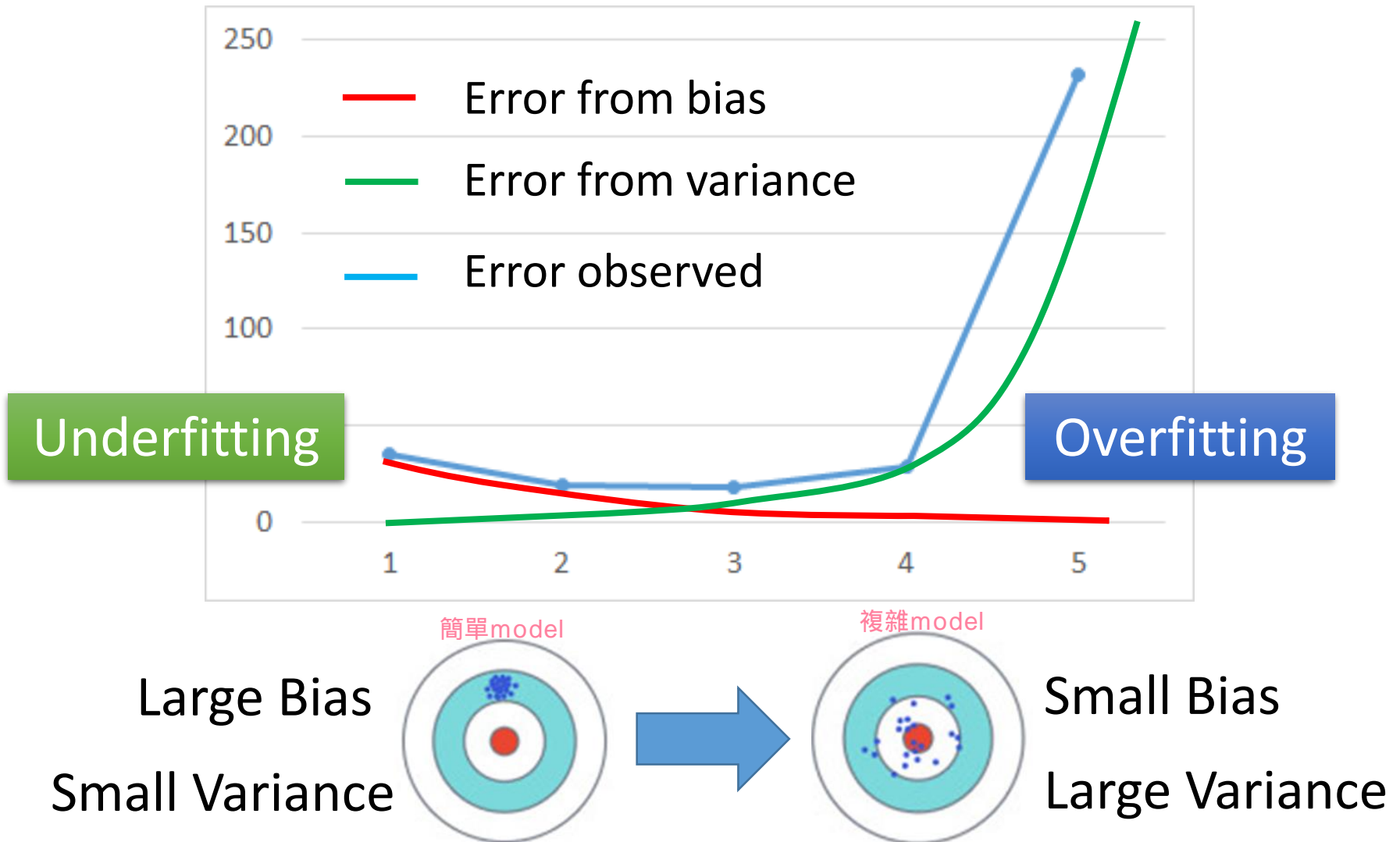
They should be diverse.

- Aggregate the classifiers (*properly*)
 - 在打王時每個人都有該站的位置

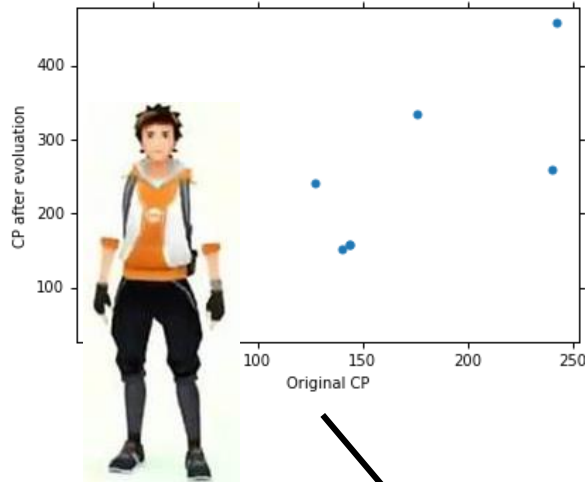
Ensemble: Bagging

用在強的model

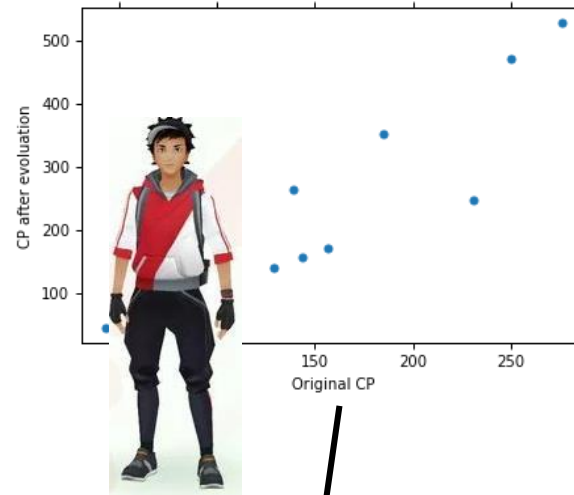
Review: Bias v.s. Variance



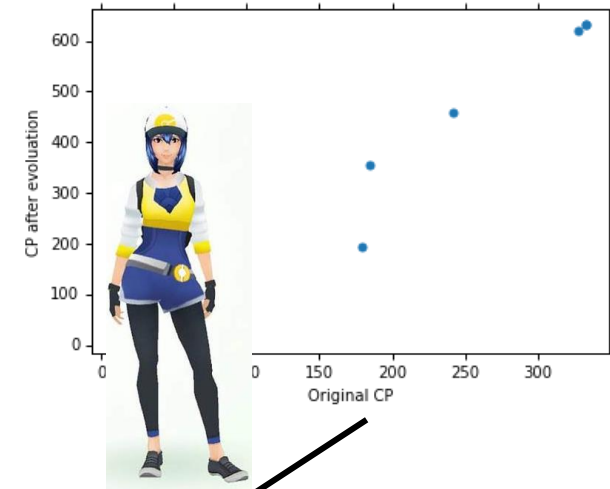
Universe 1



Universe 2

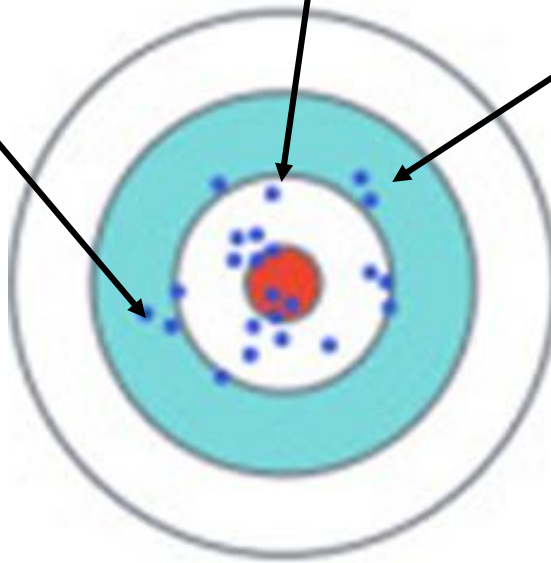


Universe 3



A complex model will have large variance.

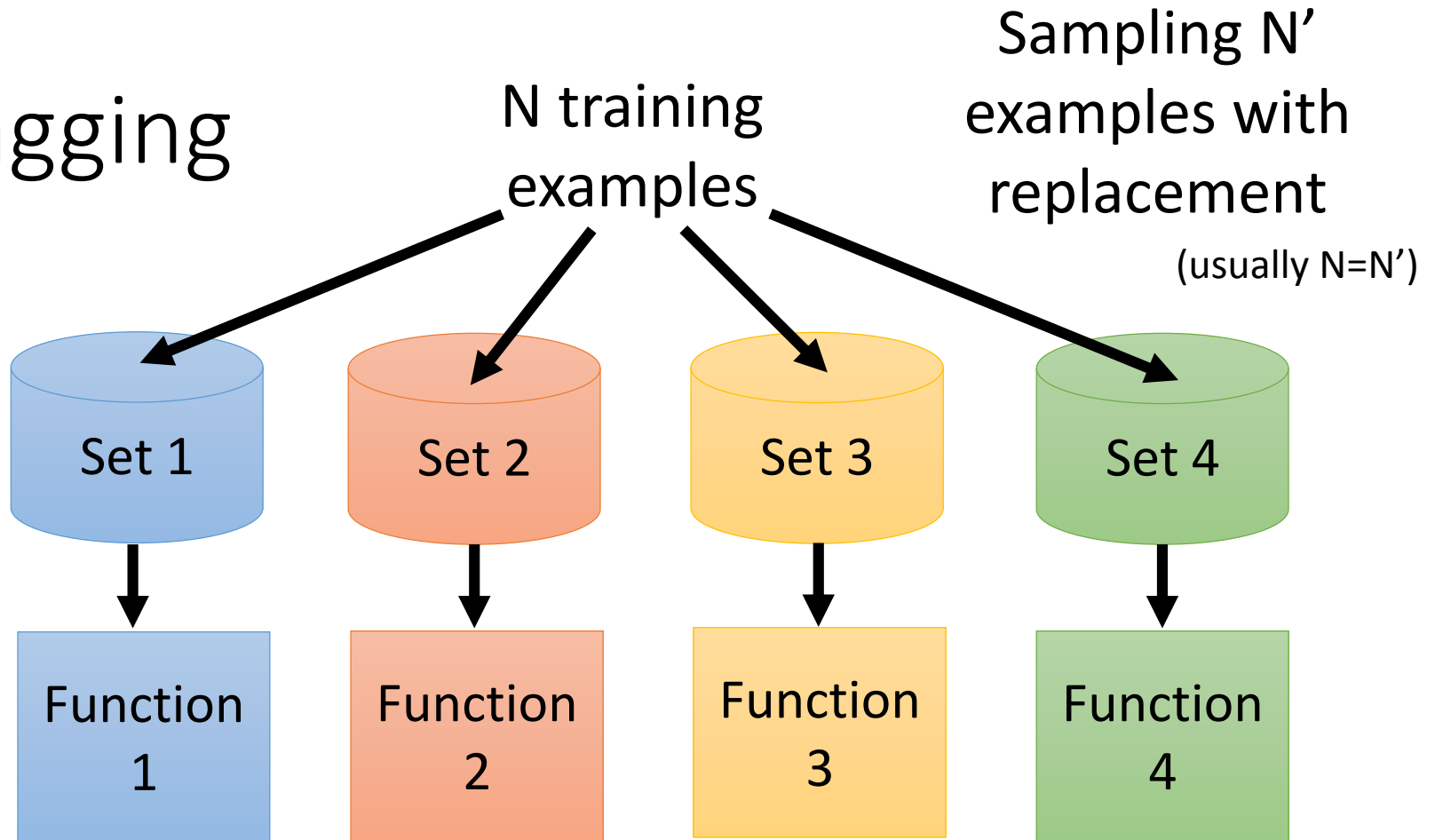
We can average complex models to reduce variance.



If we average all the f^* , is it close to \hat{f}

$$E[f^*] = \hat{f}$$

Bagging



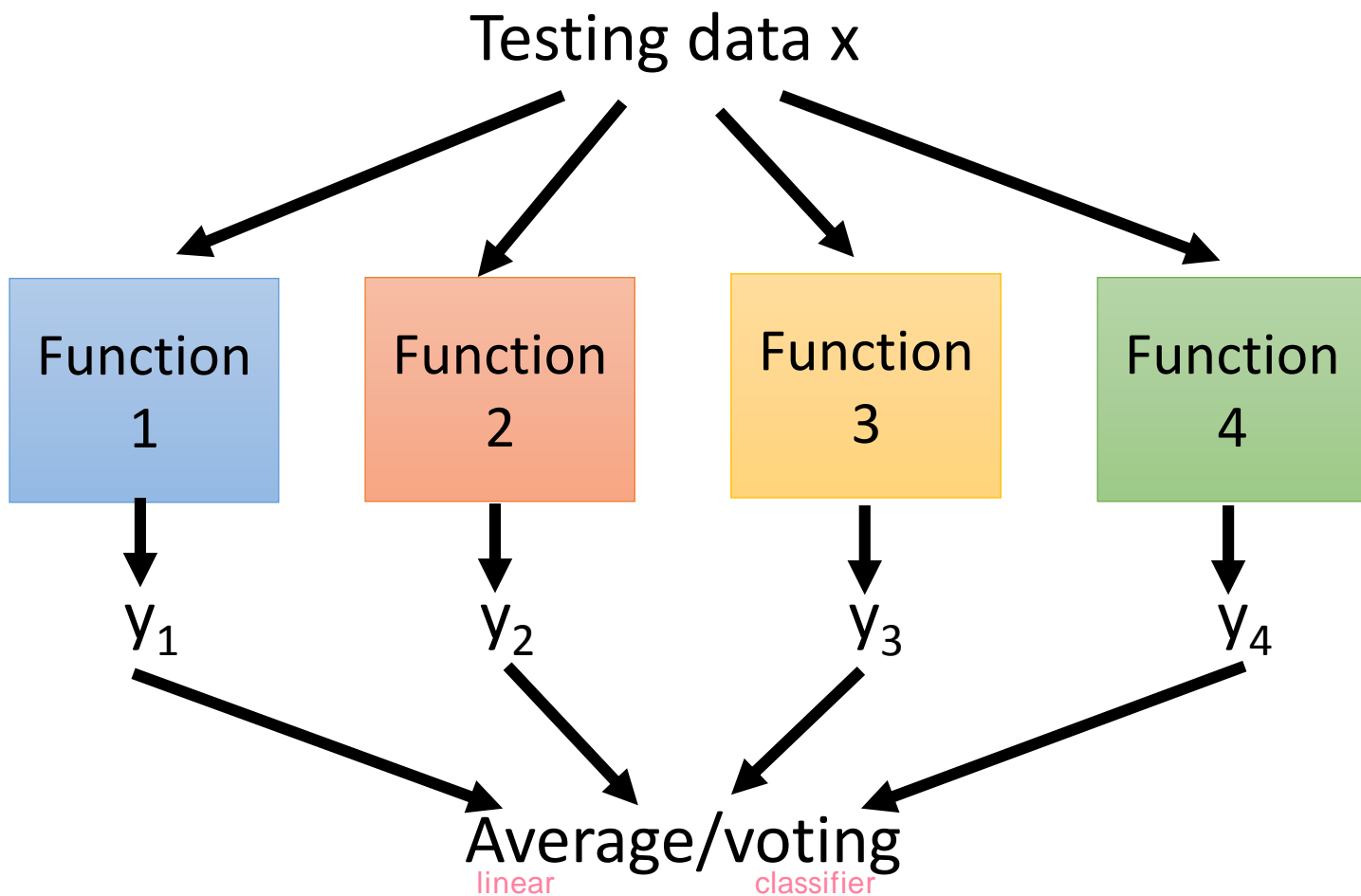
Bagging

This approach would be helpful when your model is complex, easy to overfit.

bagging目的在減低variance

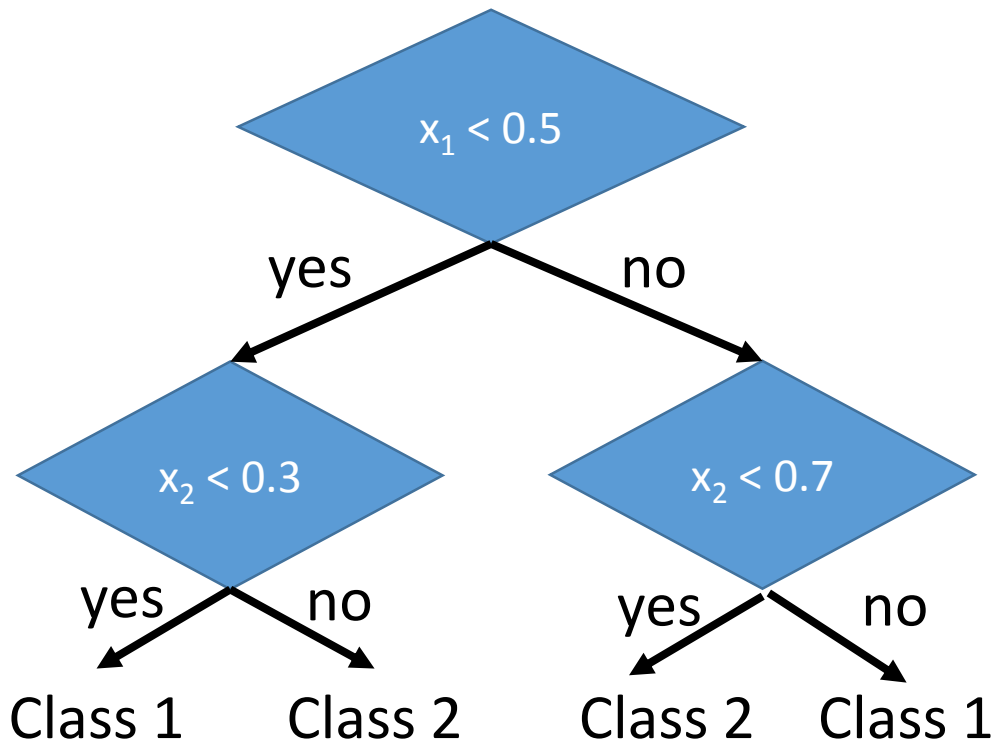
e.g. decision tree

random forest就是decision tree做bagging的版本

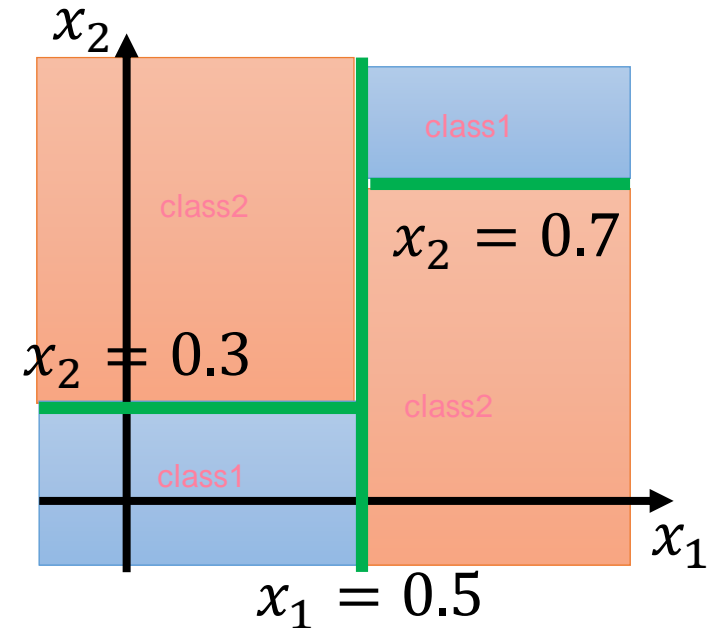


Decision Tree

Assume each object x is represented by a 2-dim vector $\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$



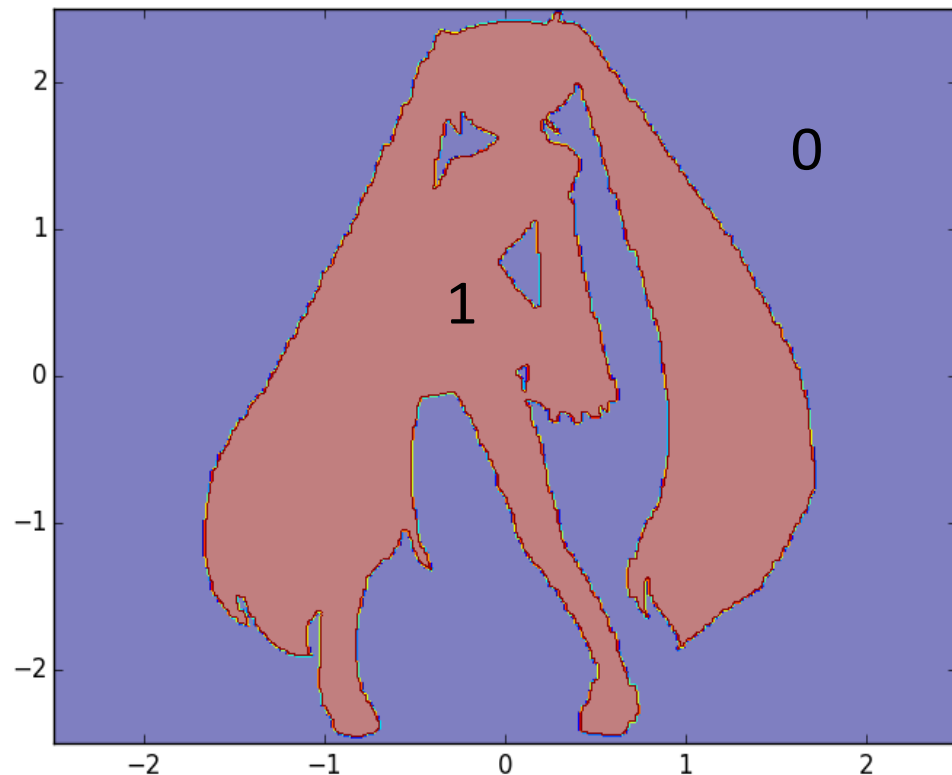
Can have more complex questions



The questions in training

number of branches,
Branching criteria,
termination criteria,
base hypothesis

Experiment: Function of Miku

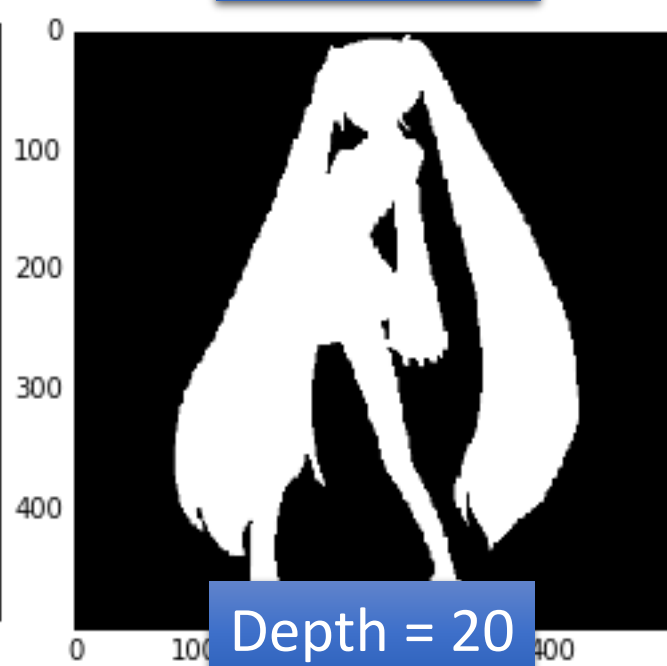
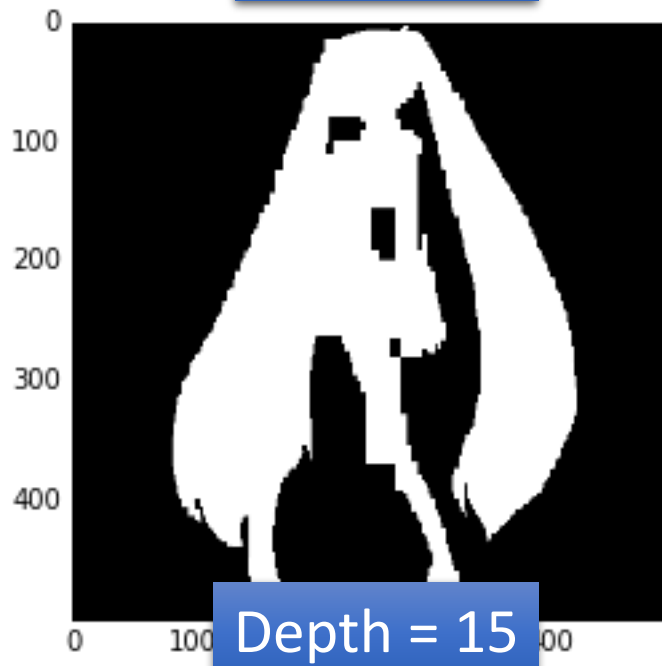
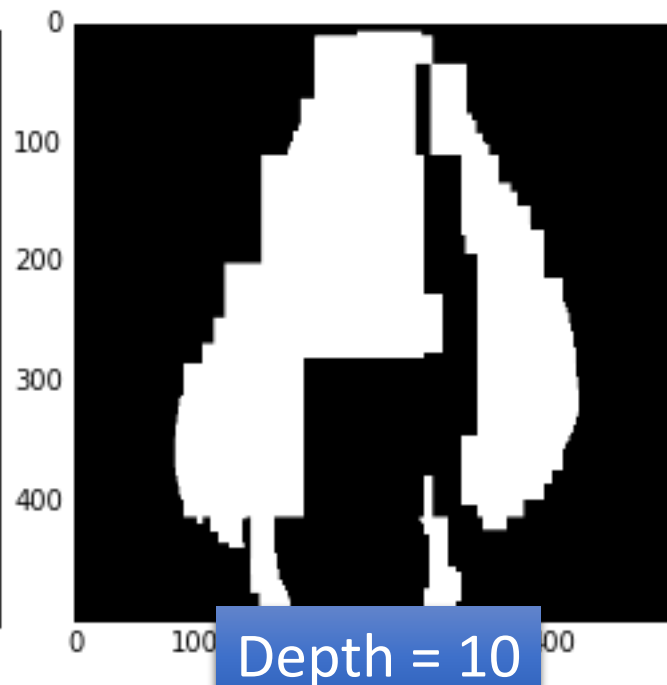
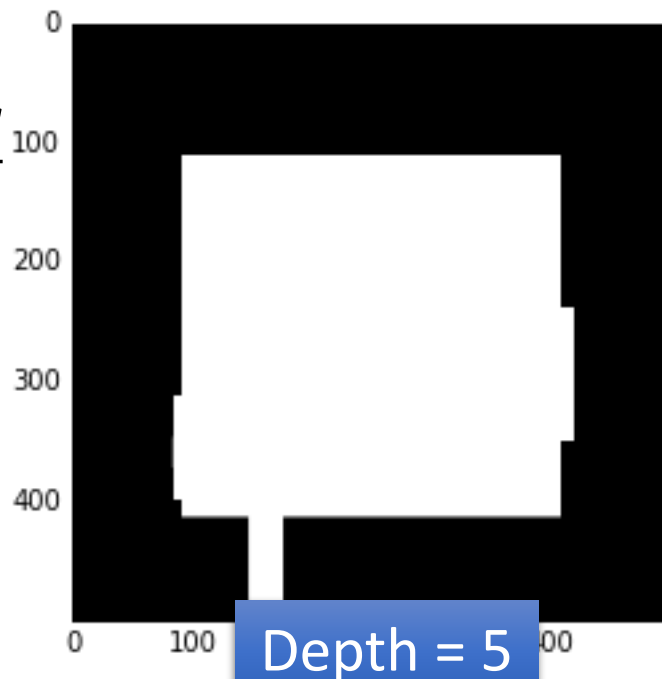


http://speech.ee.ntu.edu.tw/~tlkagk/courses/MLDS_2015_2/theano/miku

(1st column: x, 2nd column: y, 3rd column: output (1 or 0))

Experiment:
Function of Miku

Single
Decision
Tree



Random Forest

train	f_1	f_2	f_3	f_4
x^1	O	X	O	X
x^2	O	X	X	O
x^3	X	O	O	X
x^4	X	O	X	O

- Decision tree:
 - Easy to achieve 0% error rate on training data
 - If each training example has its own leaf
- Random forest: Bagging of decision tree
 - Resampling training data is not sufficient
 - Randomly restrict the features/questions used in each split

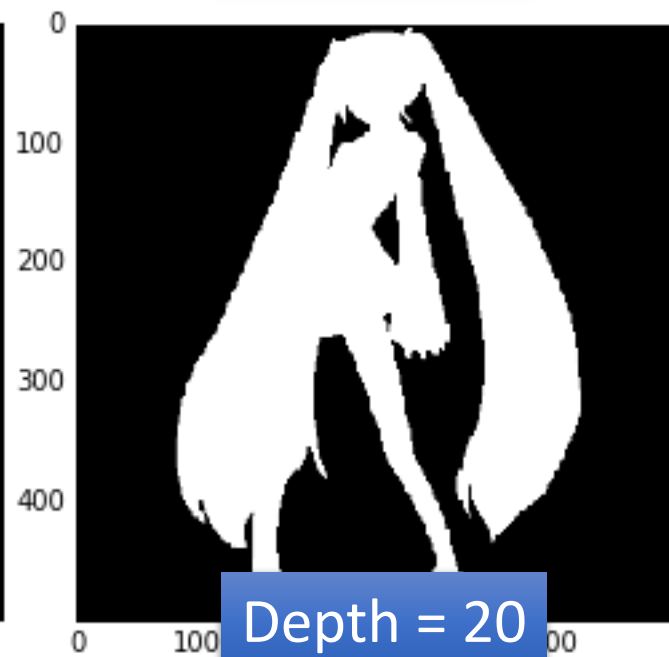
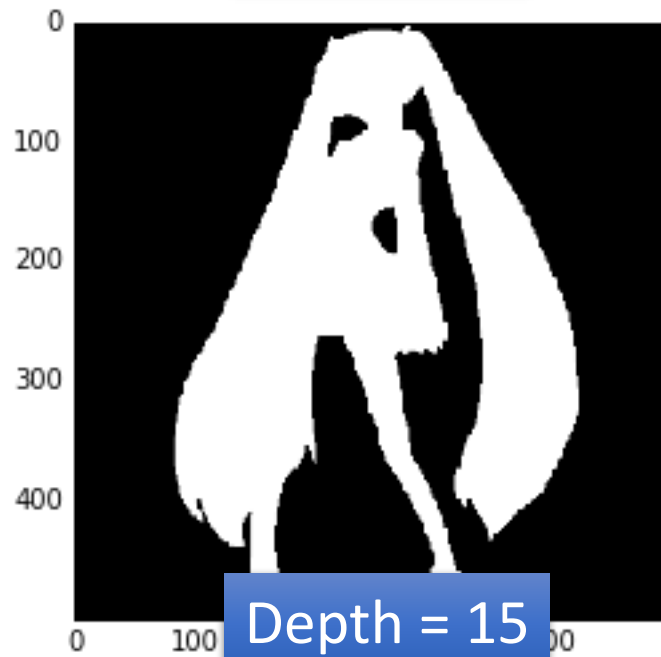
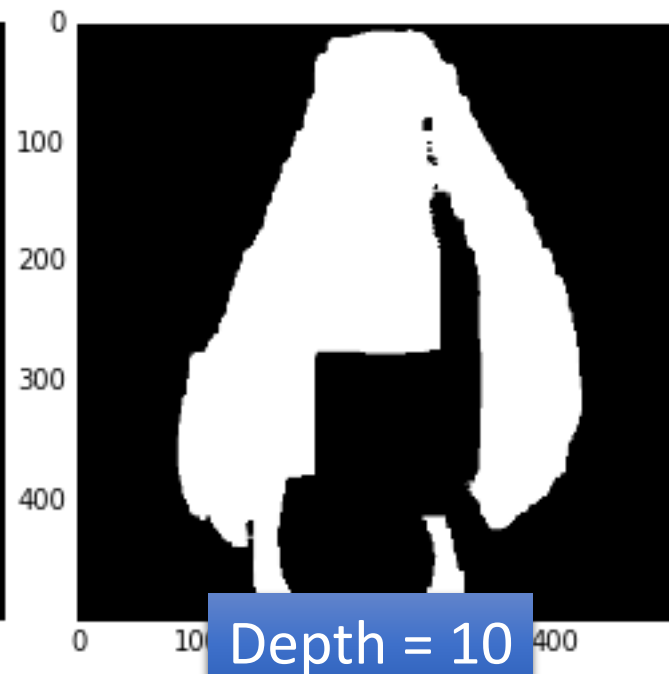
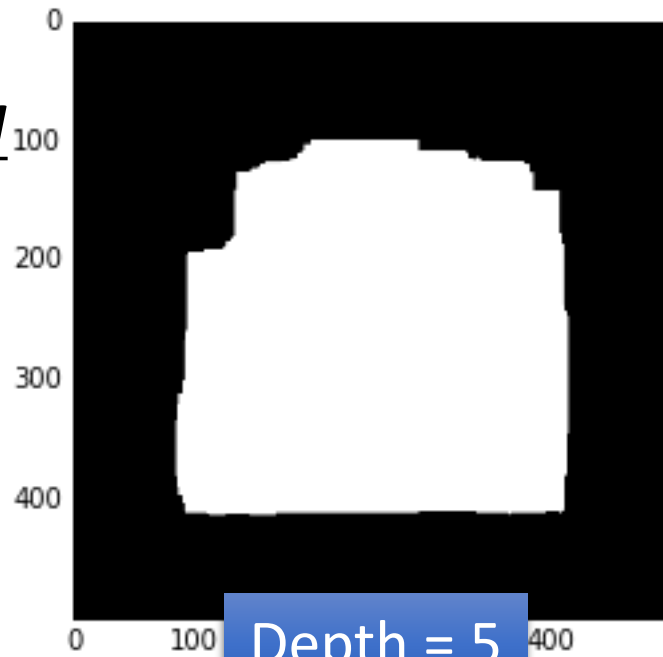
在分branch時, random決定哪些feature或問題是不能用的
- Out-of-bag validation for bagging
 - Using RF = $f_2 + f_4$ to test x^1
 - Using RF = $f_2 + f_3$ to test x^2
 - Using RF = $f_1 + f_4$ to test x^3
 - Using RF = $f_1 + f_3$ to test x^4

Out-of-bag (OOB) error
Good error estimation
of testing set

Experiment:
Function of Miku

Random
Forest

(100 trees)



Ensemble: Boosting

Improving Weak Classifiers

用在弱的model

Boosting

Training data:

$$\{(x^1, \hat{y}^1), \dots, (x^n, \hat{y}^n), \dots, (x^N, \hat{y}^N)\}$$

$\hat{y} = \pm 1$ (binary classification)

- Guarantee:
 - If your ML algorithm can produce classifier with error rate smaller than 50% on training data
 - You can obtain 0% error rate classifier after boosting.
- Framework of boosting
 - Obtain the first classifier $f_1(x)$
 - Find another function $f_2(x)$ to help $f_1(x)$
 - However, if $f_2(x)$ is similar to $f_1(x)$, it will not help a lot. $f_1(x)$ 和 $f_2(x)$ 的特性要是互補的
 - We want $f_2(x)$ to be complementary with $f_1(x)$ (How?)
 - Obtain the second classifier $f_2(x)$
 - Finally, combining all the classifiers
- The classifiers are learned sequentially. 訓練是有順序的

How to obtain different classifiers?

- Training on different training data sets
- How to have different training data sets
 - Re-sampling your training data to form a new set
 - Re-weighting your training data to form a new set
 - In real implementation, you only have to change the cost/objective function

改weight製造出新的dataset

$$(x^1, \hat{y}^1, u^1) \quad u^1 = \cancel{1} \quad 0.4$$

$$(x^2, \hat{y}^2, u^2) \quad u^2 = \cancel{1} \quad 2.1$$

$$(x^3, \hat{y}^3, u^3) \quad u^3 = \cancel{1} \quad 0.7$$

↑
每一筆data的weight

$$L(f) = \sum_n l(f(x^n), \hat{y}^n)$$



$$L(f) = \sum_n u^n l(f(x^n), \hat{y}^n)$$

Idea of Adaboost

- Idea: **training $f_2(x)$ on the new training set that fails $f_1(x)$**
- How to find a new training set that fails $f_1(x)$?

ε_1 : the error rate of $f_1(x)$ on its training data

$$\varepsilon_1 = \frac{\sum_n u_1^n \delta(f_1(x^n) \neq \hat{y}^n)}{Z_1} \quad Z_1 = \sum_n u_1^n \quad \varepsilon_1 < 0.5$$

Changing the example weights from u_1^n to u_2^n such that

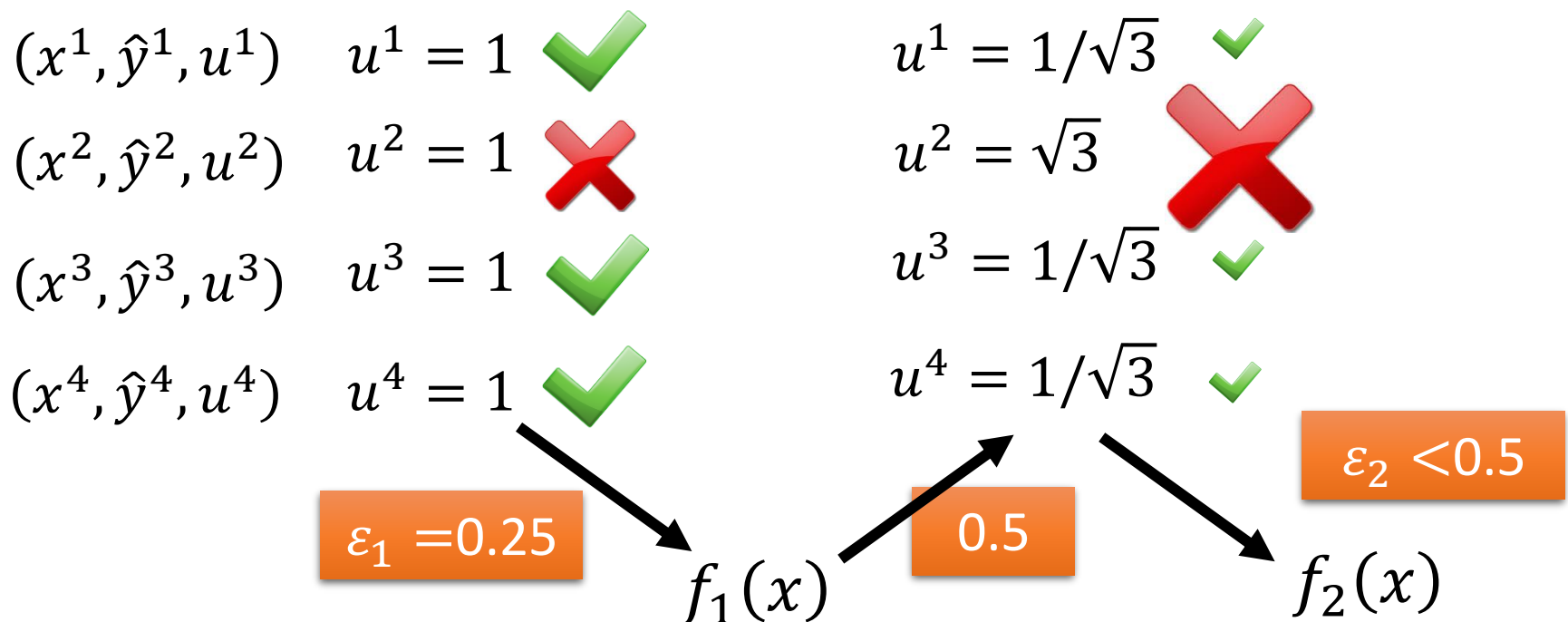
$$\frac{\sum_n u_2^n \delta(f_1(x^n) \neq \hat{y}^n)}{Z_2} = 0.5$$

The performance of f_1 for new weights would be random.

Training $f_2(x)$ based on the new weights u_2^n

Re-weighting Training Data

- Idea: training $f_2(x)$ on the new training set that fails $f_1(x)$
- How to find a new training set that fails $f_1(x)$?



Re-weighting Training Data

- Idea: **training $f_2(x)$ on the new training set that fails $f_1(x)$**
- How to find a new training set that fails $f_1(x)$?

$$\left\{ \begin{array}{ll} \text{If } x^n \text{ misclassified by } f_1 \ (f_1(x^n) \neq \hat{y}^n) & u_2^n \leftarrow u_1^n \text{ multiplying } d_1 \quad \text{increase} \\ \text{If } x^n \text{ correctly classified by } f_1 \ (f_1(x^n) = \hat{y}^n) & u_2^n \leftarrow u_1^n \text{ divided by } d_1 \quad \text{decrease} \end{array} \right.$$

f_2 will be learned based on example weights u_2^n

What is the value of d_1 ?

Re-weighting Training Data

$$\varepsilon_1 = \frac{\sum_n u_1^n \delta(f_1(x^n) \neq \hat{y}^n)}{Z_1}$$

$$Z_1 = \sum_n u_1^n$$

$$\frac{\sum_n u_2^n \delta(f_1(x^n) \neq \hat{y}^n)}{Z_2} = 0.5$$

$f_1(x^n) \neq \hat{y}^n \quad u_2^n \leftarrow u_1^n$ multiplying d_1
 $f_1(x^n) = \hat{y}^n \quad u_2^n \leftarrow u_1^n$ divided by d_1

$$= \sum_{f_1(x^n) \neq \hat{y}^n} u_1^n d_1$$

$$= \sum_{f_1(x^n) \neq \hat{y}^n} u_2^n + \sum_{f_1(x^n) = \hat{y}^n} u_2^n$$

$$= \sum_n u_2^n$$

$$= \sum_{f_1(x^n) \neq \hat{y}^n} u_1^n d_1 + \sum_{f_1(x^n) = \hat{y}^n} u_1^n / d_1$$

$$\frac{\sum_{f_1(x^n) \neq \hat{y}^n} u_1^n d_1 + \sum_{f_1(x^n) = \hat{y}^n} u_1^n / d_1}{\sum_{f_1(x^n) \neq \hat{y}^n} u_1^n d_1} = 2$$

Re-weighting Training Data

$$\varepsilon_1 = \frac{\sum_n u_1^n \delta(f_1(x^n) \neq \hat{y}^n)}{Z_1} \quad Z_1 = \sum_n u_1^n$$

$$\frac{\sum_n u_2^n \delta(f_1(x^n) \neq \hat{y}^n)}{Z_2} = 0.5 \quad \begin{array}{ll} f_1(x^n) \neq \hat{y}^n & u_2^n \leftarrow u_1^n \text{ multiplying } d_1 \\ f_1(x^n) = \hat{y}^n & u_2^n \leftarrow u_1^n \text{ divided by } d_1 \end{array}$$

$$\frac{\sum_{f_1(x^n) \neq \hat{y}^n} u_1^n d_1 + \sum_{f_1(x^n) = \hat{y}^n} u_1^n / d_1}{\sum_{f_1(x^n) \neq \hat{y}^n} u_1^n d_1} = 2 \quad \frac{\sum_{f_1(x^n) = \hat{y}^n} u_1^n / d_1}{\sum_{f_1(x^n) \neq \hat{y}^n} u_1^n d_1} = 1$$

$$\sum_{f_1(x^n) = \hat{y}^n} u_1^n / d_1 = \sum_{f_1(x^n) \neq \hat{y}^n} u_1^n d_1 \quad \frac{1}{d_1} \sum_{f_1(x^n) = \hat{y}^n} u_1^n = d_1 \sum_{f_1(x^n) \neq \hat{y}^n} u_1^n$$

$$\varepsilon_1 = \frac{\sum_{f_1(x^n) \neq \hat{y}^n} u_1^n}{Z_1} \quad \frac{Z_1(1 - \varepsilon_1)}{Z_1 \varepsilon_1}$$

$$\sum_{f_1(x^n) \neq \hat{y}^n} u_1^n = Z_1 \varepsilon_1$$

$$Z_1(1 - \varepsilon_1)/d_1 = Z_1 \varepsilon_1 d_1$$

$$d_1 = \sqrt{(1 - \varepsilon_1)/\varepsilon_1} > 1$$

Algorithm for AdaBoost

- Giving training data $\{(x^1, \hat{y}^1, u_1^1), \dots, (x^n, \hat{y}^n, u_1^n), \dots, (x^N, \hat{y}^N, u_1^N)\}$
 - $\hat{y} = \pm 1$ (Binary classification), $u_1^n = 1$ (equal weights)
 - For $t = 1, \dots, T$:
 - Training weak classifier $f_t(x)$ with weights $\{u_t^1, \dots, u_t^N\}$
 - ε_t is the error rate of $f_t(x)$ with weights $\{u_t^1, \dots, u_t^N\}$
 - For $n = 1, \dots, N$:
 - If x^n is misclassified by $f_t(x)$: $\hat{y}^n \neq f_t(x^n)$
 - $u_{t+1}^n = u_t^n \times d_t = u_t^n \times \exp(\alpha_t)$ $d_t = \sqrt{(1 - \varepsilon_t)/\varepsilon_t}$
 - Else:
 - $u_{t+1}^n = u_t^n / d_t = u_t^n \times \exp(-\alpha_t)$ $\alpha_t = \ln \sqrt{(1 - \varepsilon_t)/\varepsilon_t}$
- $$u_{t+1}^n \leftarrow u_t^n \times \exp(-\alpha_t)$$

Algorithm for AdaBoost

- We obtain a set of functions: $f_1(x), \dots, f_t(x), \dots, f_T(x)$
- How to aggregate them?
 - Uniform weight:
 - $H(x) = \text{sign}(\sum_{t=1}^T f_t(x))$
 - Non-uniform weight:
 - $H(x) = \text{sign}(\sum_{t=1}^T \alpha_t f_t(x))$

Smaller error ε_t ,
larger weight for
final voting

$$\alpha_t = \ln \sqrt{(1 - \varepsilon_t) / \varepsilon_t}$$

$$\varepsilon_t = 0.1$$

$$\varepsilon_t = 0.4$$

$$u_{t+1}^n = u_t^n \times \exp(-\hat{y}^n f_t(x^n) \alpha_t)$$

$$\alpha_t = 1.10$$

$$\alpha_t = 0.20$$

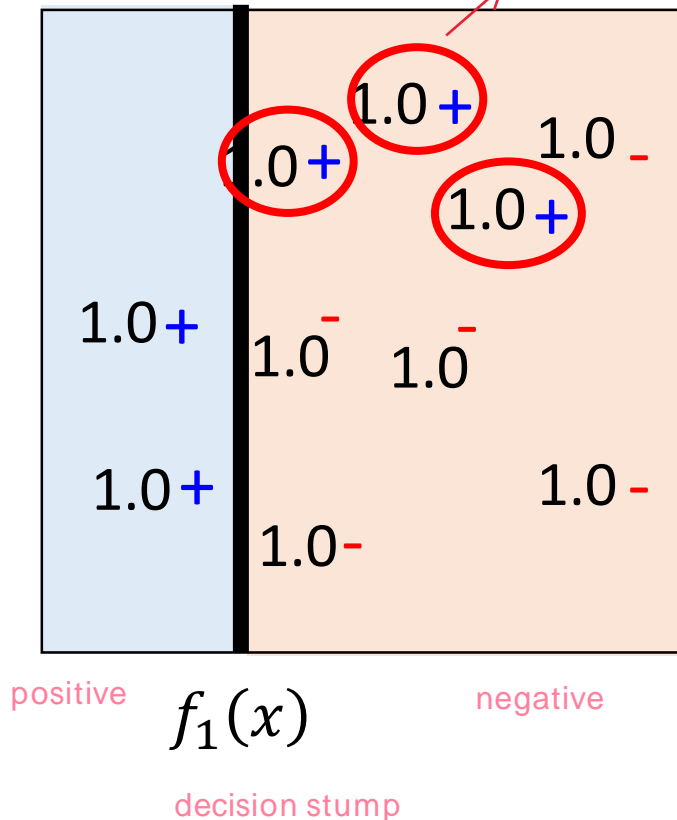
Toy Example

$T=3$, weak classifier = decision stump

• $t=1$

weight=1

三筆data分類錯



error rate

$$\epsilon_1 = 0.30$$

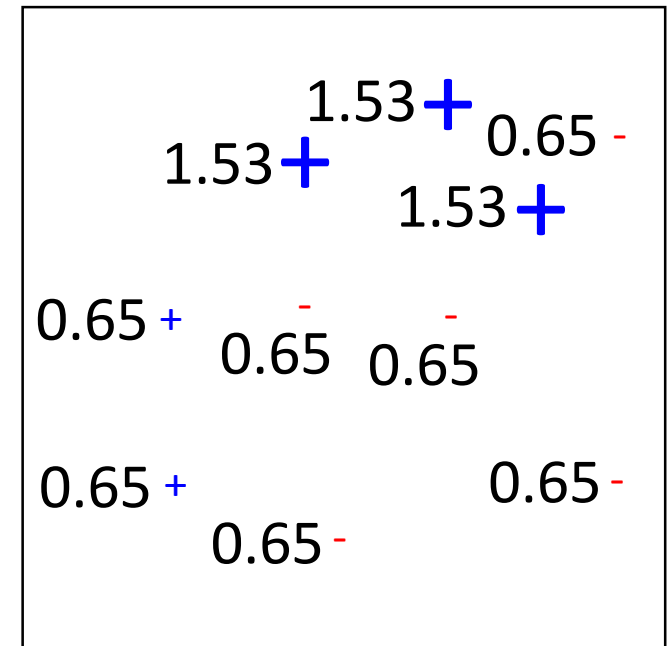
$$d_1 = 1.53$$

$$\alpha_1 = 0.42$$

改weight:

分類正確 \rightarrow weight變小

分類錯誤 \rightarrow weight變大



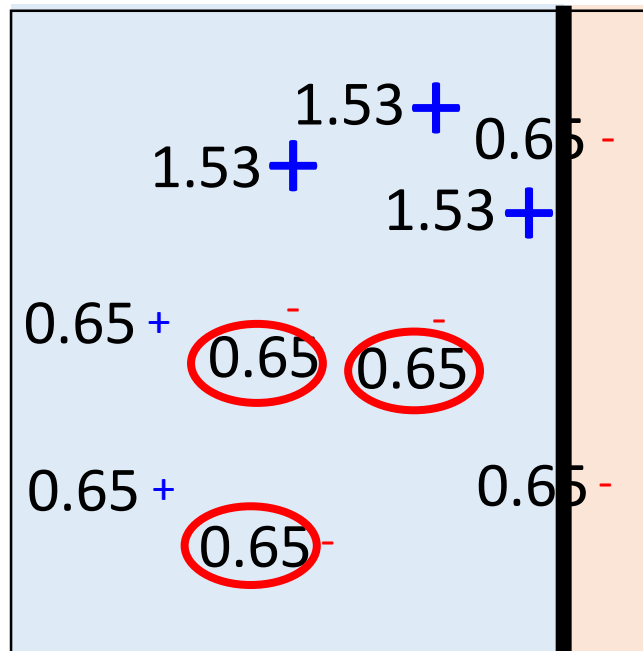
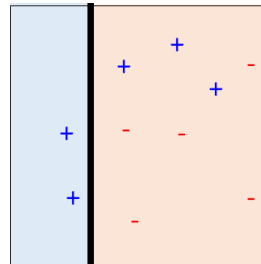
Toy Example

$T=3$, weak classifier = decision stump

• $t=2$

$$f_1(x):$$

$$\alpha_1 = 0.42$$



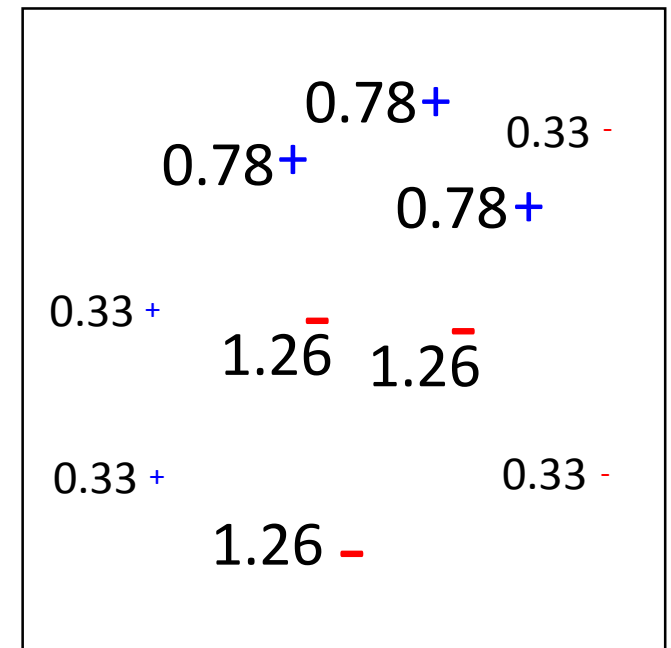
$$f_2(x)$$



$$\varepsilon_2 = 0.21$$

$$d_2 = 1.94$$

$$\alpha_2 = 0.66$$



再找decision stump

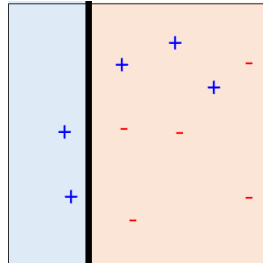
Toy Example

$T=3$, weak classifier = decision stump

• $t=3$

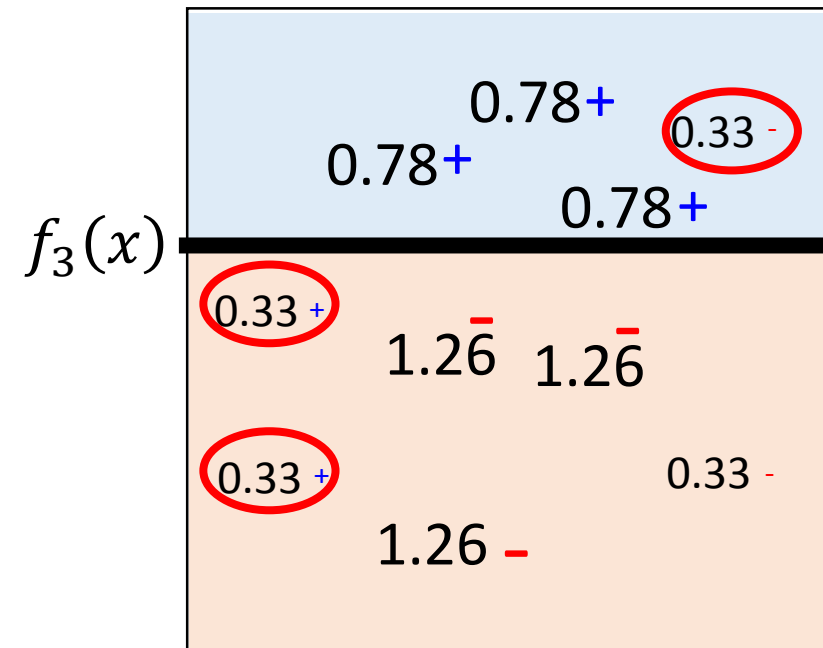
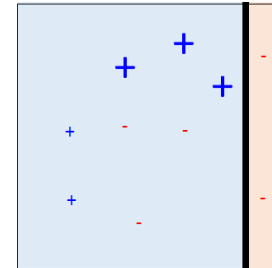
$f_1(x)$:

$$\alpha_1 = 0.42$$



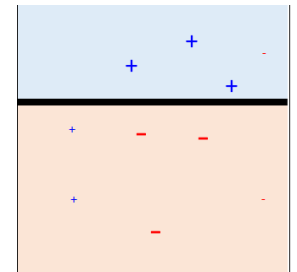
$f_2(x)$:

$$\alpha_2 = 0.66$$



$f_3(x)$:

$$\alpha_3 = 0.95$$



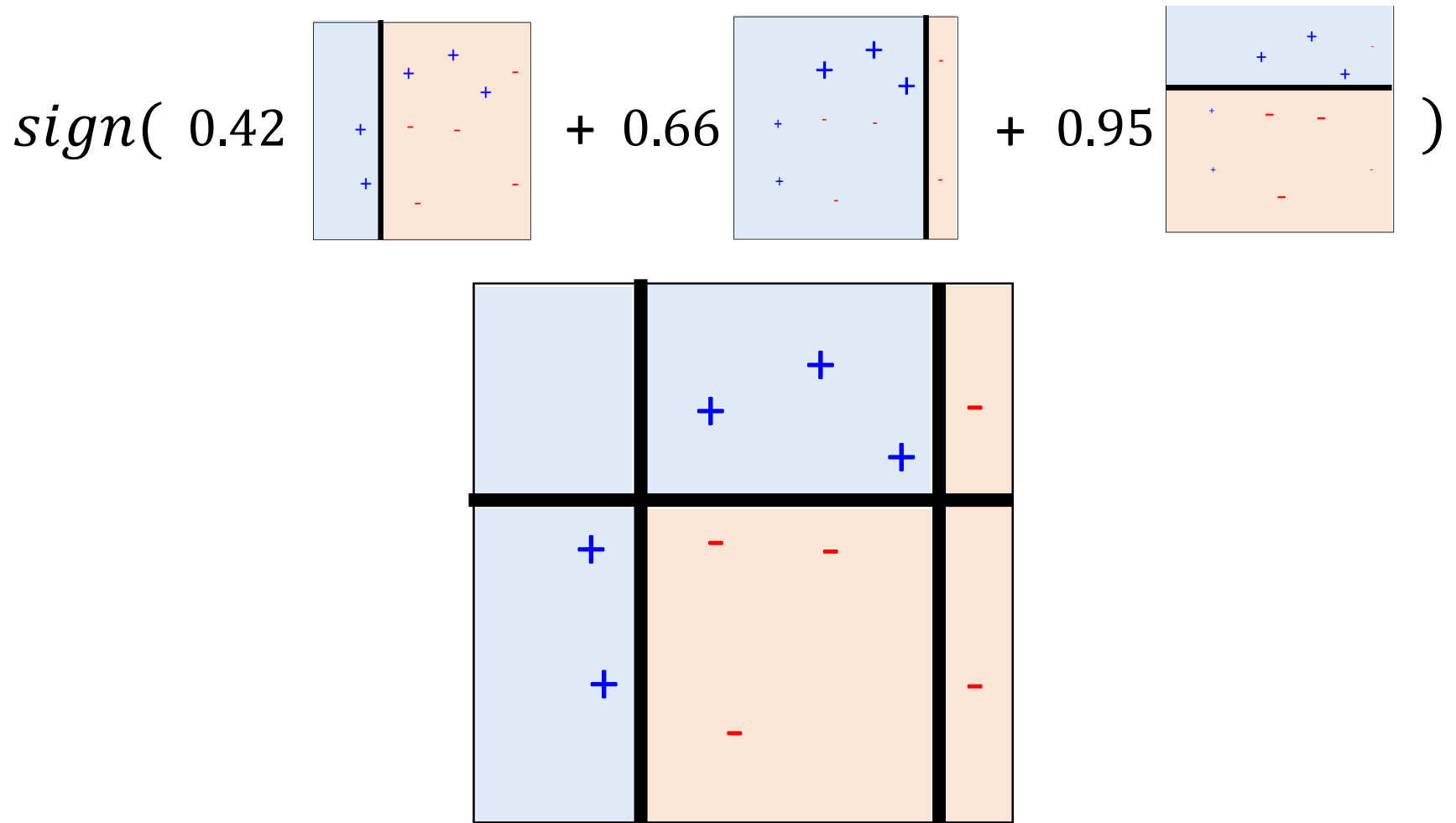
$$\varepsilon_3 = 0.13$$

$$d_3 = 2.59$$

$$\alpha_3 = 0.95$$

Toy Example

- Final Classifier: $H(x) = \text{sign}(\sum_{t=1}^T \alpha_t f_t(x))$



Warning of Math

$$H(x) = \text{sign} \left(\sum_{t=1}^T \alpha_t f_t(x) \right) \quad \alpha_t = \ln \sqrt{(1 - \varepsilon_t) / \varepsilon_t}$$

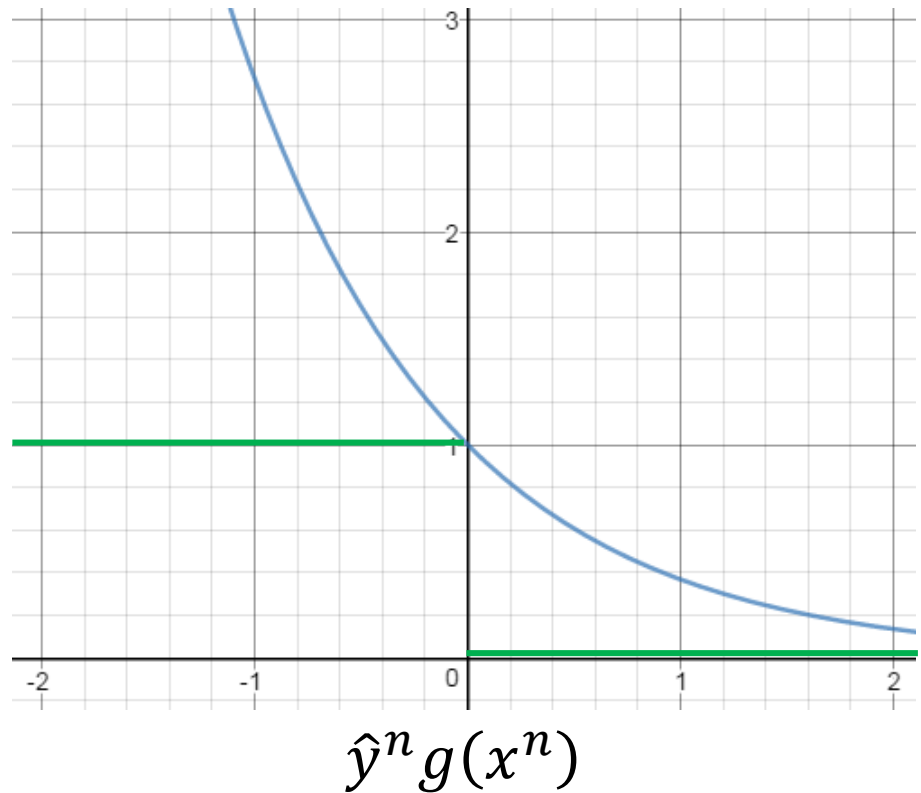
As we have more and more f_t (T increases), $H(x)$ achieves smaller and smaller error rate on training data.

Error Rate of Final Classifier

- Final classifier: $H(x) = \text{sign}(\sum_{t=1}^T \alpha_t f_t(x))$
 - $\alpha_t = \ln \sqrt{(1 - \varepsilon_t) / \varepsilon_t}$

Training Data Error Rate

$$\begin{aligned} &= \frac{1}{N} \sum_n \delta(H(x^n) \neq \hat{y}^n) \\ &= \frac{1}{N} \sum_n \delta(\hat{y}^n g(x^n) < 0) \\ &\leq \frac{1}{N} \sum_n \exp(-\hat{y}^n g(x^n)) \end{aligned}$$



Training Data Error Rate

$$\leq \frac{1}{N} \sum_n \exp(-\hat{y}^n g(x^n)) = \frac{1}{N} Z_{T+1}$$

$$g(x) = \sum_{t=1}^T \alpha_t f_t(x)$$

$$\alpha_t = \ln \sqrt{(1 - \varepsilon_t) / \varepsilon_t}$$

Z_t : the summation of the weights of training data for training f_t

What is Z_{T+1} =? $Z_{T+1} = \sum_n u_{T+1}^n$

$$\left. \begin{array}{l} u_1^n = 1 \\ u_{t+1}^n = u_t^n \times \exp(-\hat{y}^n f_t(x^n) \alpha_t) \end{array} \right\} u_{T+1}^n = \prod_{t=1}^T \exp(-\hat{y}^n f_t(x^n) \alpha_t)$$

$$\begin{aligned} Z_{T+1} &= \sum_n \prod_{t=1}^T \exp(-\hat{y}^n f_t(x^n) \alpha_t) \\ &= \sum_n \exp \left(-\hat{y}^n \sum_{t=1}^T f_t(x^n) \alpha_t \right) \end{aligned}$$

Training Data Error Rate

$$\leq \frac{1}{N} \sum_n \exp(-\hat{y}^n g(x^n)) = \frac{1}{N} Z_{T+1}$$

$$g(x) = \sum_{t=1}^T \alpha_t f_t(x)$$

$$\alpha_t = \ln \sqrt{(1 - \epsilon_t) / \epsilon_t}$$

$$Z_1 = N \quad (\text{equal weights})$$

$$Z_t = \underline{Z_{t-1} \epsilon_t} \exp(\alpha_t) + \underline{Z_{t-1} (1 - \epsilon_t)} \exp(-\alpha_t)$$

Misclassified portion in Z_{t-1}

Correctly classified portion in Z_{t-1}

$$= Z_{t-1} \epsilon_t \sqrt{(1 - \epsilon_t) / \epsilon_t} + Z_{t-1} (1 - \epsilon_t) \sqrt{\epsilon_t / (1 - \epsilon_t)}$$

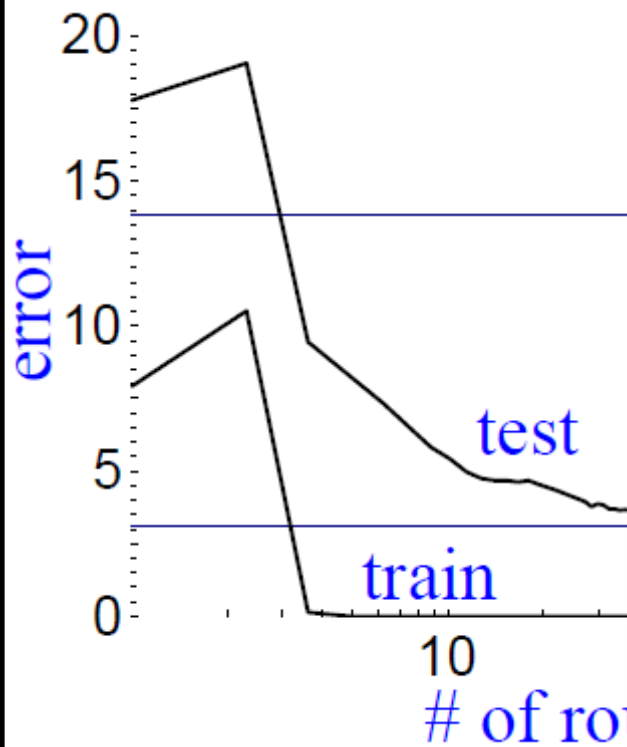
$$= Z_{t-1} \times 2\sqrt{\epsilon_t (1 - \epsilon_t)} \quad Z_{T+1} = N \prod_{t=1}^T 2\sqrt{\epsilon_t (1 - \epsilon_t)}$$

$$\text{Training Data Error Rate} \leq \prod_{t=1}^T \underline{2\sqrt{\epsilon_t (1 - \epsilon_t)}}_{<1}$$

Smaller and
smaller

End of Warning

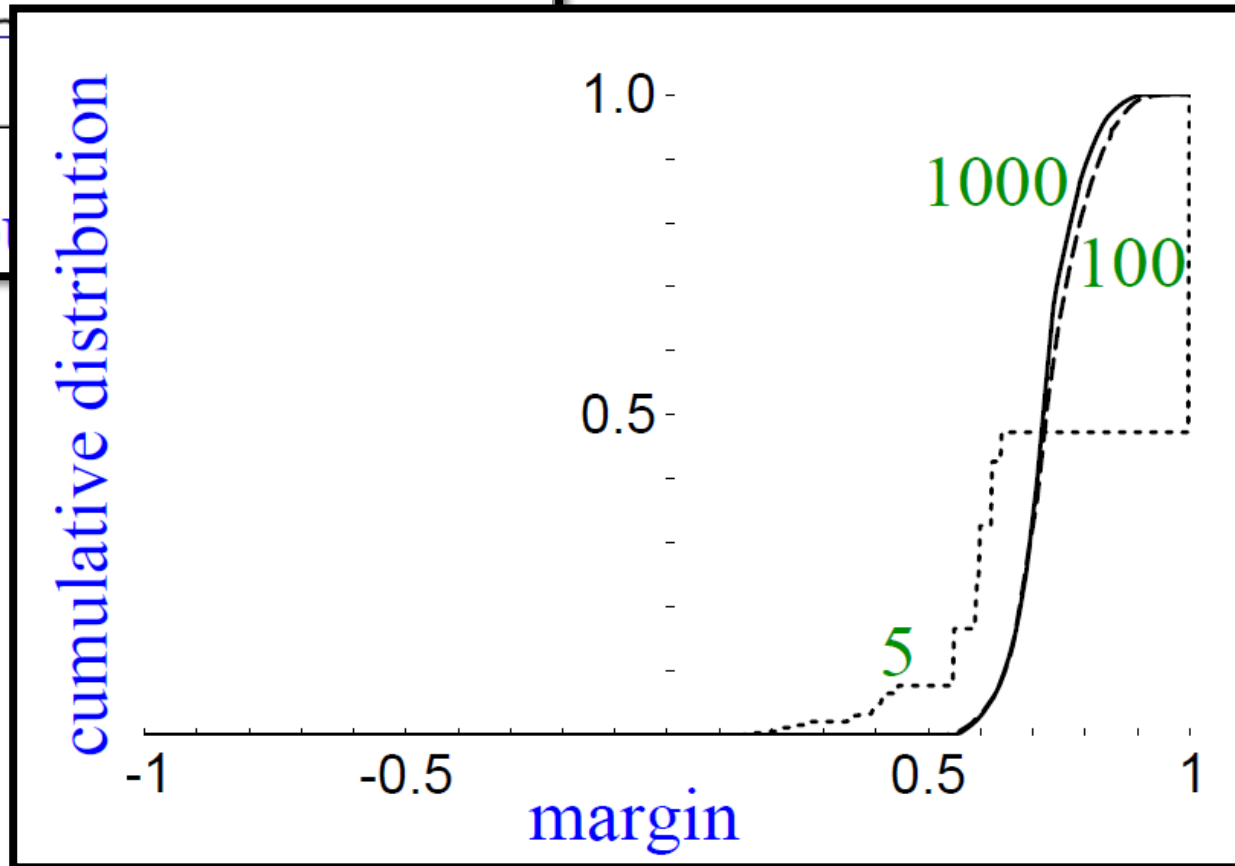
Even though the training error is 0, the testing error still decreases?



$$H(x) = \text{sign} \left(\sum_{t=1}^T \alpha_t f_t(x) \right)$$

$g(x)$

Margin = $\hat{y}g(x)$



Large Margin?

$$H(x) = \text{sign} \left(\underbrace{\sum_{t=1}^T \alpha_t f_t(x)}_{g(x)} \right)$$

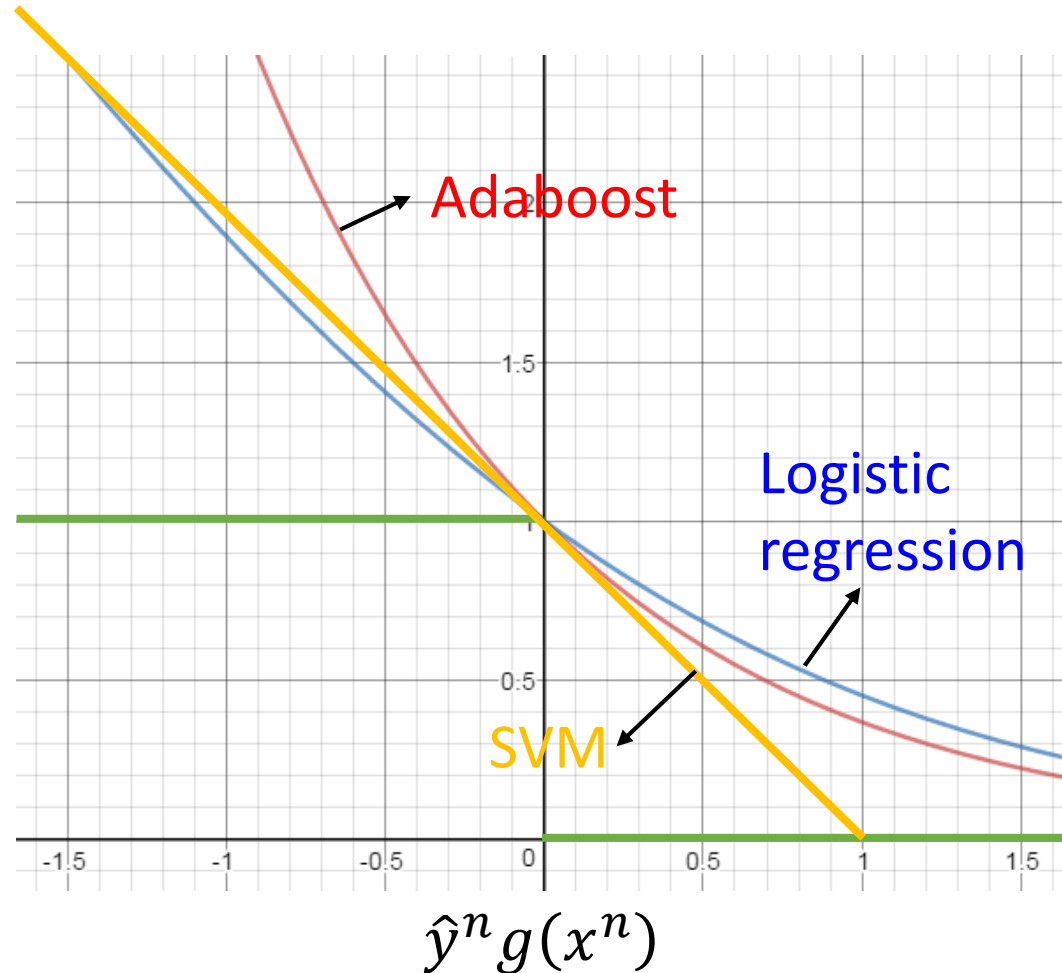
Training Data Error Rate =

$$= \frac{1}{N} \sum_n \delta(H(x^n) \neq \hat{y}^n)$$

$$\leq \frac{1}{N} \sum_n \exp(-\hat{y}^n g(x^n))$$

$$= \prod_{t=1}^T 2\sqrt{\epsilon_t(1-\epsilon_t)}$$

Getting smaller and smaller as T increase

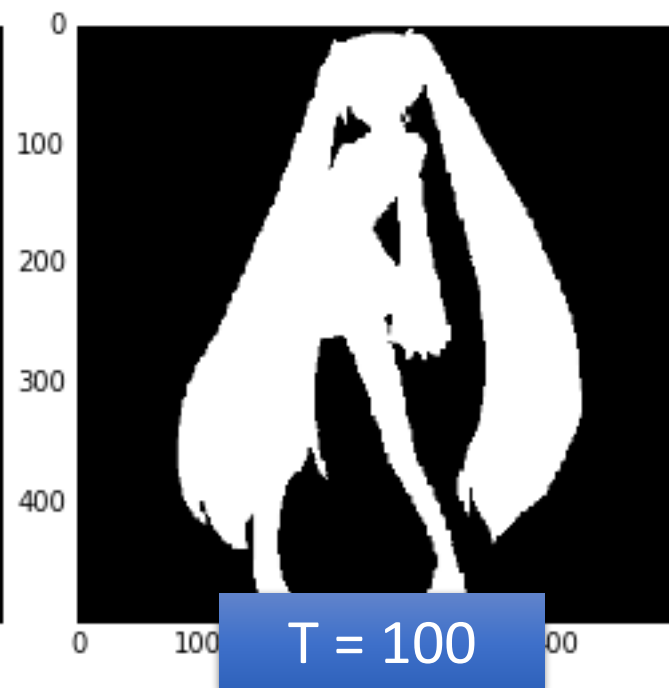
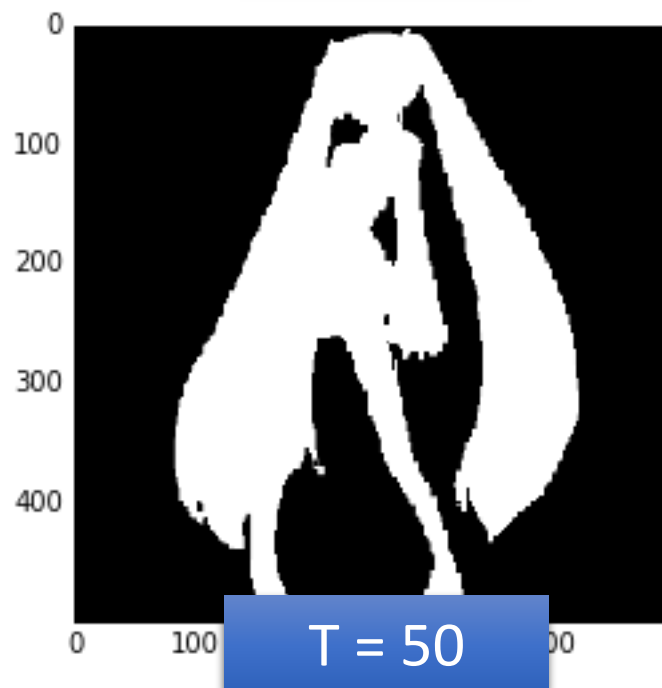
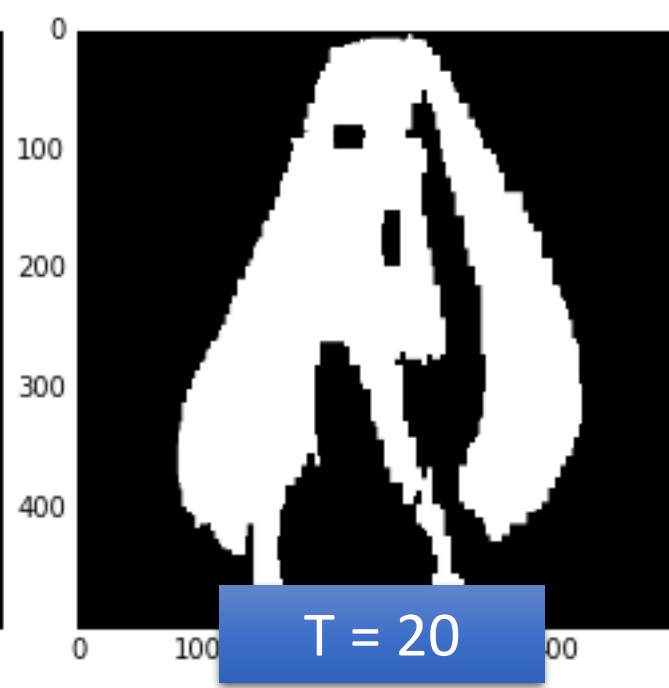
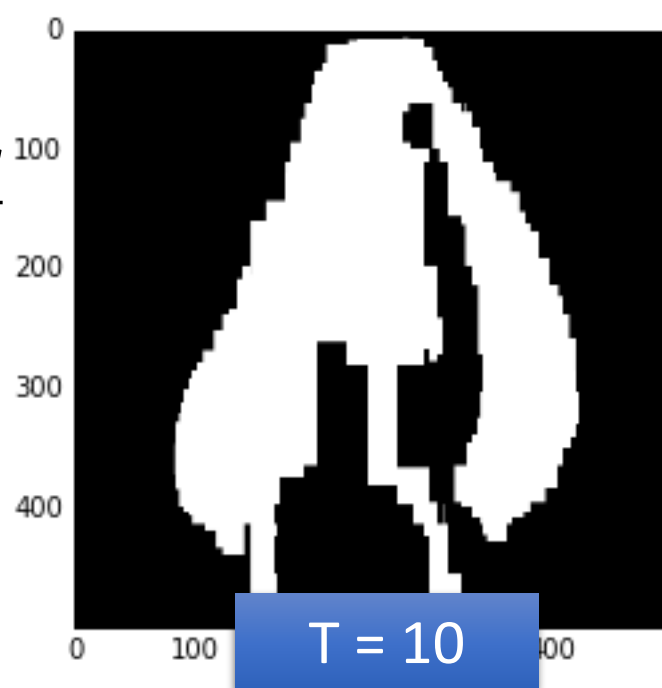


Experiment: Function of Miku

Adaboost
+Decision Tree

這些樹枝之間是互補的

(depth = 5)



To learn more ...

- Introduction of Adaboost:
 - Freund; Schapire (1999). "A Short Introduction to Boosting"
- Multiclass/Regression
 - Y. Freund, R. Schapire, "A Decision-Theoretic Generalization of on-Line Learning and an Application to Boosting", 1995.
 - Robert E. Schapire and Yoram Singer. Improved boosting algorithms using confidence-rated predictions. In Proceedings of the Eleventh Annual Conference on Computational Learning Theory, pages 80–91, 1998.
- Gentle Boost
 - Schapire, Robert; Singer, Yoram (1999). "Improved Boosting Algorithms Using Confidence-rated Predictions".

General Formulation of Boosting

- Initial function $g_0(x) = 0$
- For $t = 1$ to T :
 - Find a function $f_t(x)$ and α_t to improve $g_{t-1}(x)$
 - $g_{t-1}(x) = \sum_{i=1}^{t-1} \alpha_i f_i(x)$
 - $g_t(x) = g_{t-1}(x) + \alpha_t f_t(x)$
- Output: $H(x) = \text{sign}(g_T(x))$

What is the learning target of $g(x)$?

$$\text{Minimize } L(g) = \sum_n l(\hat{y}^n, g(x^n)) = \sum_n \exp(-\hat{y}^n g(x^n))$$

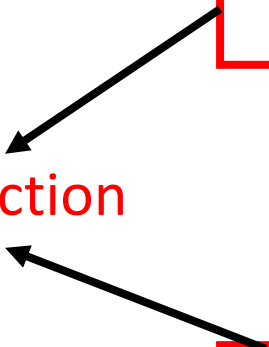
Gradient Boosting

- Find $g(x)$, minimize $L(g) = \sum_n \exp(-\hat{y}^n g(x^n))$
 - If we already have $g(x) = g_{t-1}(x)$, how to update $g(x)$?

Gradient Descent:

$$g_t(x) = g_{t-1}(x) - \eta \left. \frac{\partial L(g)}{\partial g(x)} \right|_{g(x) = g_{t-1}(x)}$$

Same direction

$$\sum_n \exp(-\hat{y}^n g_{t-1}(x^n)) (-\hat{y}^n)$$
$$g_t(x) = g_{t-1}(x) + \alpha_t f_t(x)$$


Gradient Boosting

$$f_t(x) \xleftrightarrow{\text{Same direction}} \sum_n \exp(-\hat{y}^n g_t(x^n)) (\hat{y}^n)$$

We want to find $f_t(x)$ maximizing

$$\sum_n \underbrace{\exp(-\hat{y}^n g_{t-1}(x^n))}_{\text{example weight } u_t^n} \underbrace{(\hat{y}^n) f_t(x^n)}_{\text{Minimize Error Same sign}}$$

$$u_t^n = \exp(-\hat{y}^n g_{t-1}(x^n)) = \exp\left(-\hat{y}^n \sum_{i=1}^{t-1} \alpha_i f_i(x^n)\right)$$

$$= \prod_{i=1}^{t-1} \exp(-\hat{y}^n \alpha_i f_i(x^n))$$

Exactly the weights we obtain in Adaboost

Gradient Boosting

- Find $g(x)$, minimize $L(g) = \sum_n \exp(-\hat{y}^n g(x^n))$

$$g_t(x) = g_{t-1}(x) + \alpha_t f_t(x)$$

α_t is something like
learning rate

Find α_t minimizing $L(g_{t+1})$

$$L(g) = \sum_n \exp(-\hat{y}^n (g_{t-1}(x) + \alpha_t f_t(x)))$$

$$= \sum_n \exp(-\hat{y}^n g_{t-1}(x)) \exp(-\hat{y}^n \alpha_t f_t(x))$$

$$= \sum_{\hat{y}^n \neq f_t(x)} \exp(-\hat{y}^n g_{t-1}(x^n)) \exp(\alpha_t) + \sum_{\hat{y}^n = f_t(x)} \exp(-\hat{y}^n g_{t-1}(x^n)) \exp(-\alpha_t)$$

Find α_t
such that

$$\frac{\partial L(g)}{\partial \alpha_t} = 0$$

$$\alpha_t = \ln \sqrt{(1 - \varepsilon_t) / \varepsilon_t}$$

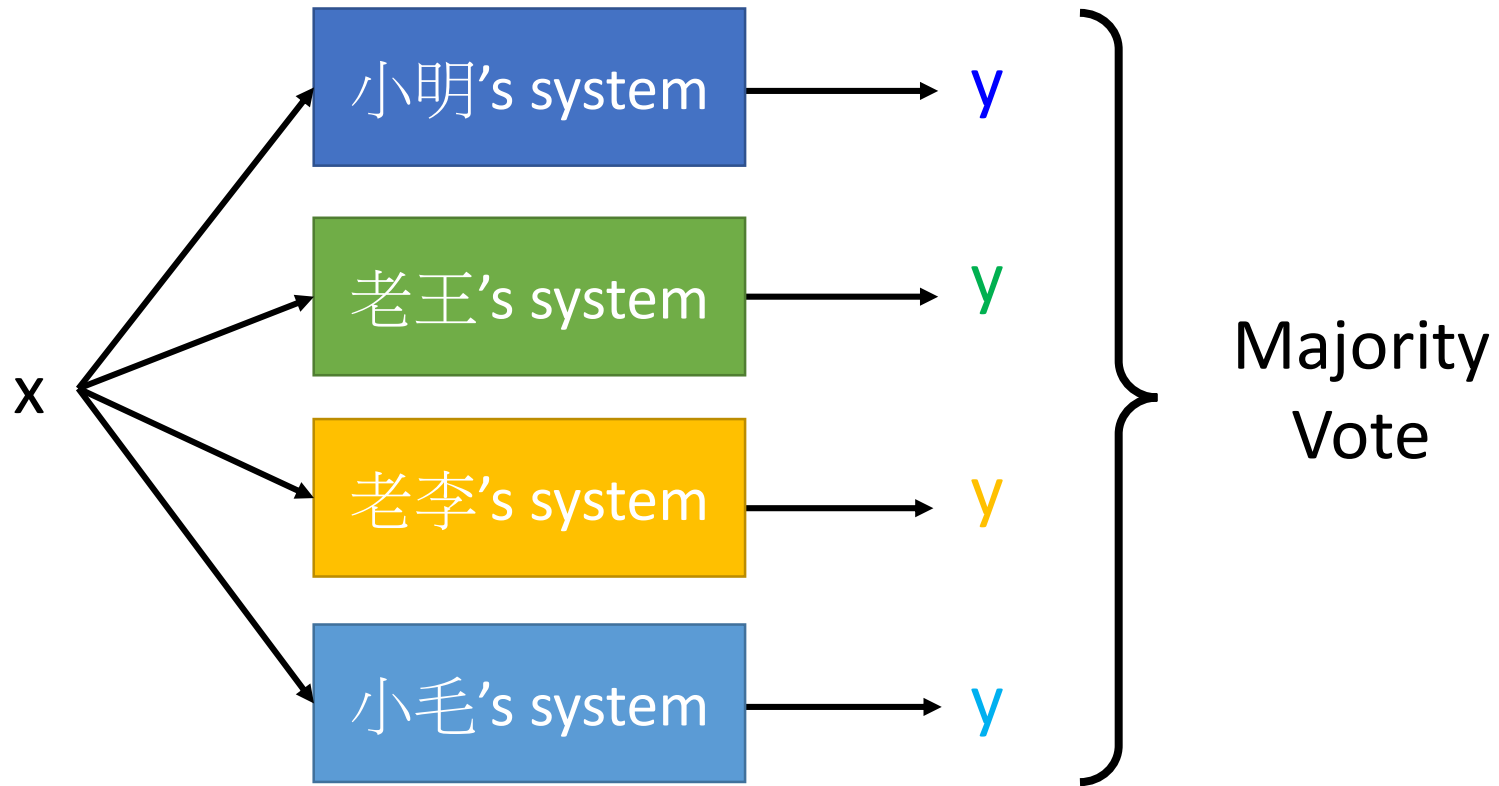
Adaboost!

Cool Demo

- http://arogozhnikov.github.io/2016/07/05/gradient_boosting_playground.html

Ensemble: Stacking

Voting



Stacking

