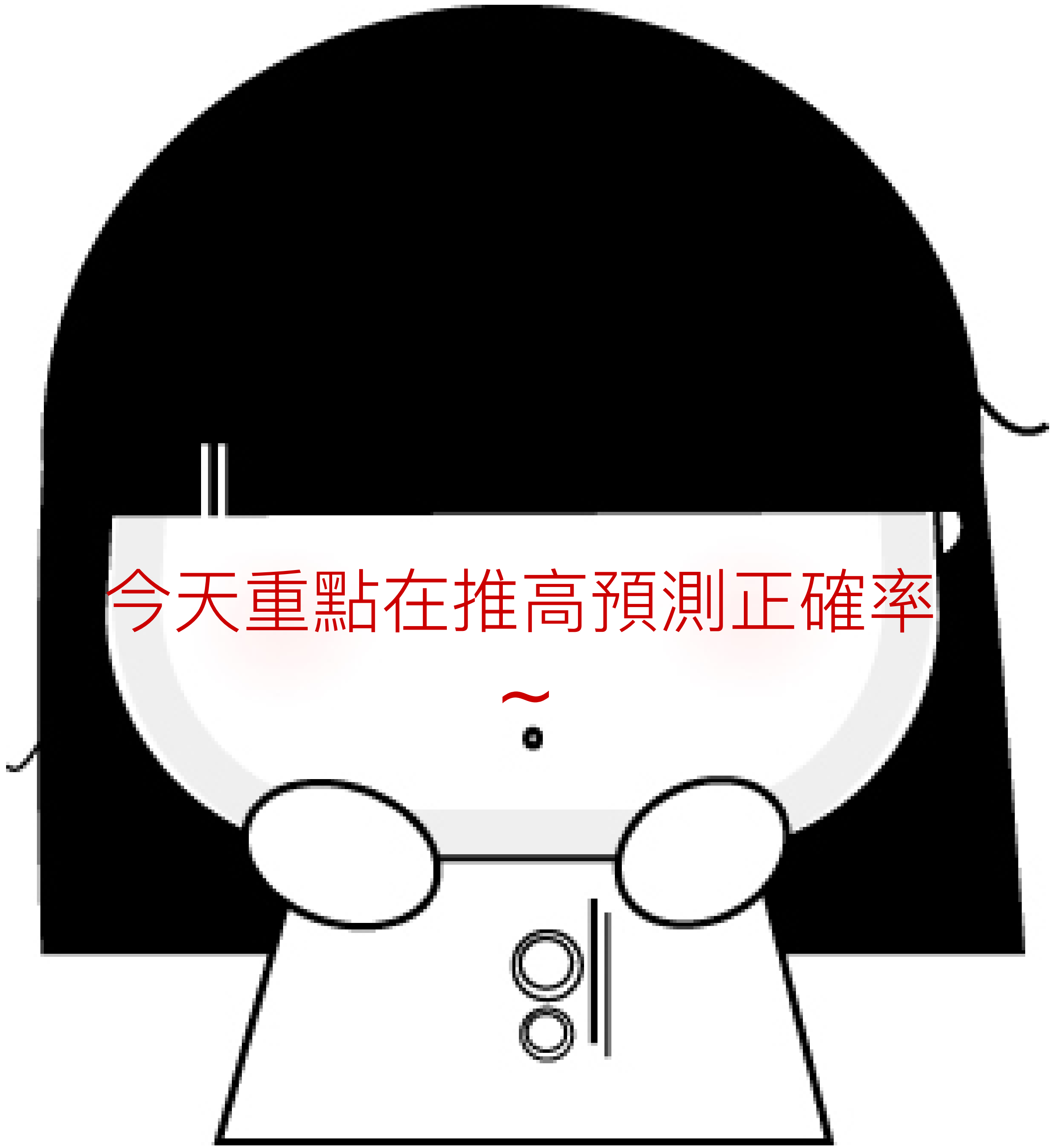
心理與神經資訊學
(Psychoinformatics & Neuroinformatics)

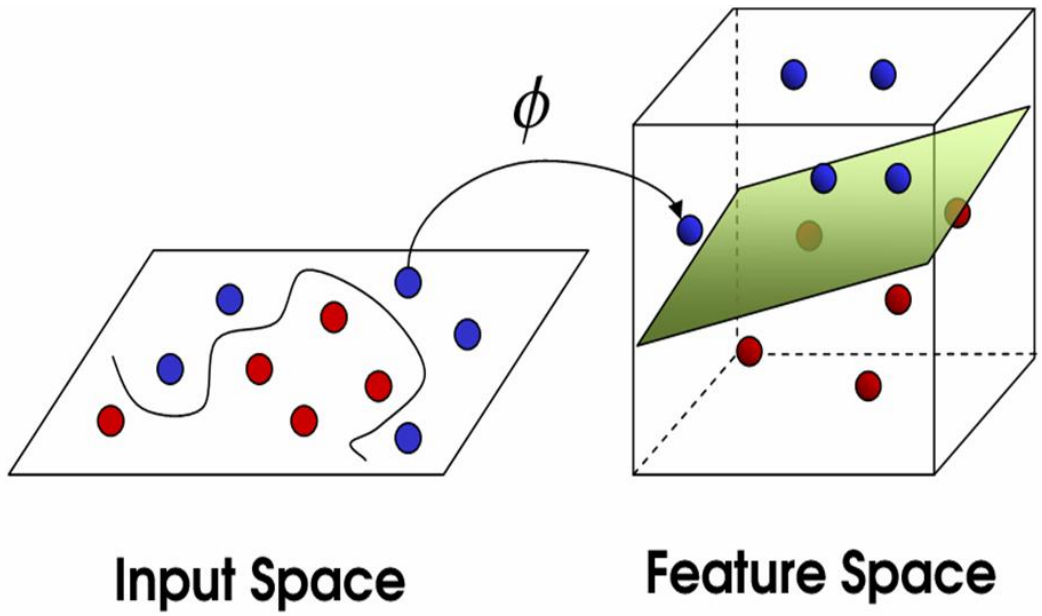
課號：Psy5261　　教室： 博雅 101
識別碼：227U9340　　時間： 四 234

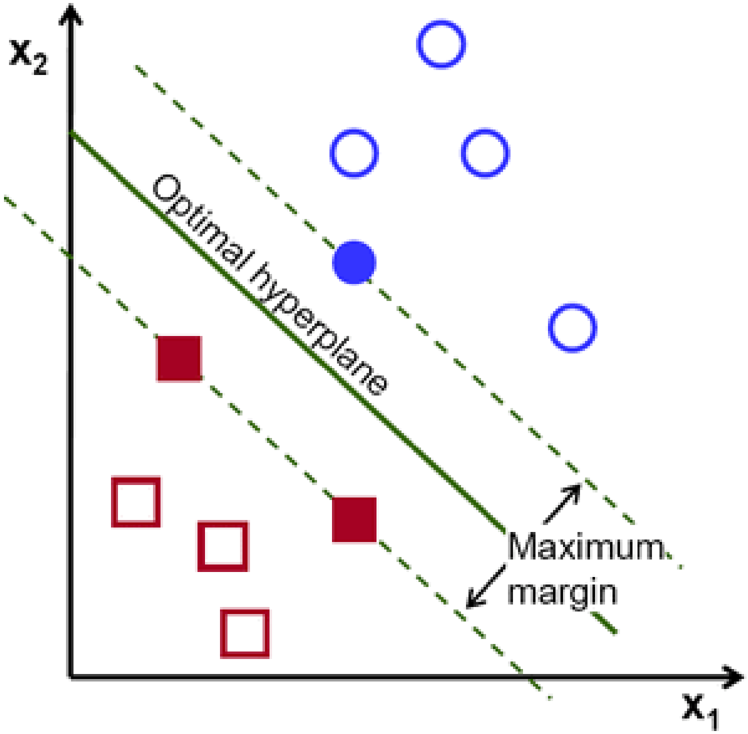
黃從仁


今天重點在推高預測正確率~

監督式學習
(Supervised Learning)

Support Vector Machine

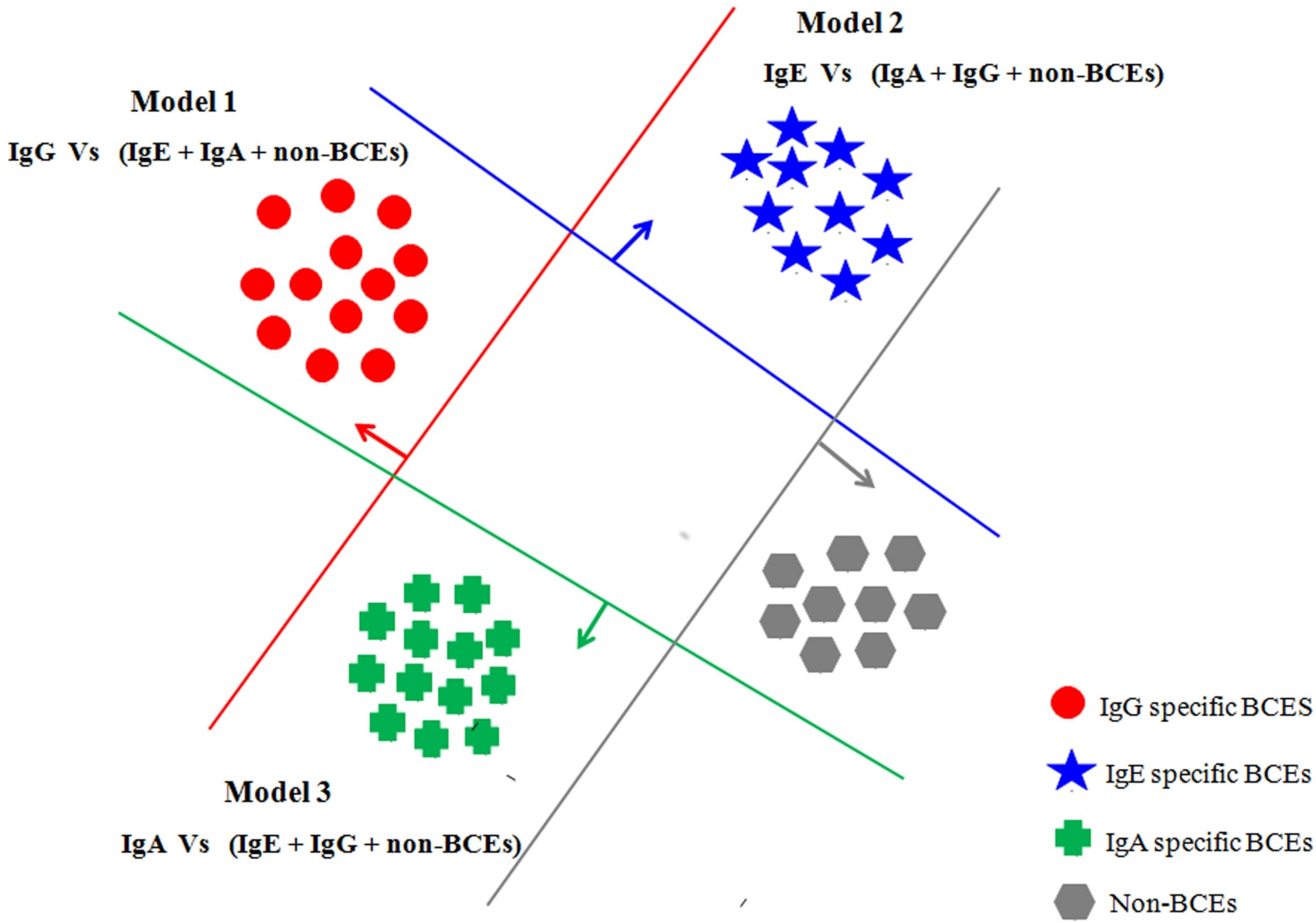





```
from sklearn import *
clf=svm.SVC()
clf.fit(X,Y) #training
print(np.mean(clf.predict(X)==Y)) #testing
```

Multiclass Classification

One vs. One 比 One vs. All 均衡但費時



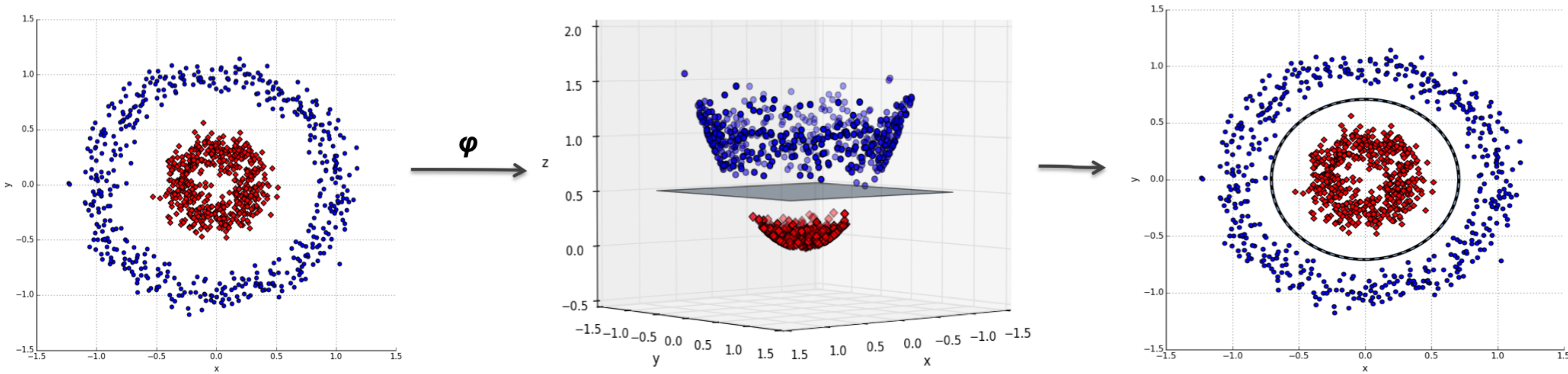
Multilabel Classification

又稱為 multi-output classification

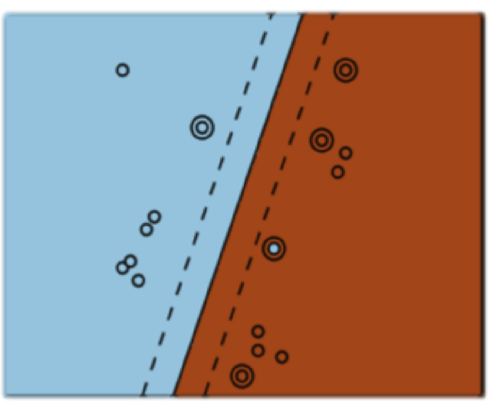
Images			
Labels	**tree water black picture** **drawing sea art blue** **boat green city**	**man woman people hair** **girl picture smile group** **photo kid family**	**sky tree water white** **house window wood sea** **ocean cloud blue door**
MLR-GL	*man white* **black** *woman people* **blue green** *red* **tree** *girl* *sky* **water** *hair* **picture** *old* *brown grass yellow face mountain*	**man woman** *black white* **people** *blue green red* **girl** *tree* **hair** *sky water* **picture** *old* *brown face yellow grass* **smile**	*man black* **white** *woman* **blue** *people green red girl* **tree** **sky** *hair* **water** *picture old* *brown yellow face grass* **window**
LIBSVM	*book smile gray sun flag* *computer brick man yellow street* *machine* **sea** *leaf road ocean* *couple forest fly purple toy*	**man hair** *black movie face* *food fire boy* **smile** *lady* *metal statue dance couple red* *table toy arm bike gold*	*building* **sky** *fence floor church* *shirt legs wall money glass* *ship room couple word city* *bald door guy orange chart*
LIBSVM+Platt	*book man smile white* **blue** *sky* **black** *woman red* **green** *people* **tree water** *computer girl* *face old hair yellow leaf*	*movie food* **man hair** *white* **smile woman** *blue face black* **people** *green red* **girl** *fire* *tree sky boy table eye*	*building* **sky** *man red floor* **white** *black woman* **blue** *church* *fence people green hair* **tree** *face shirt room grass chart*
MLR-L1	**tree green** *hair movie white* **black** *people grass statue leaf* *orange old bike red flower* *mountain* **picture** *dance eye dirt*	**hair** *tree black movie green* **man** *eye* **woman** *white hand* *face* **girl people smile** *dance* *red hat orange statue brown*	**tree** *hair movie black* **white** *green square people eye* **blue** *dance hand hat orange logo* *wall red statue man bike*

HyperParameters

邊界的位置是 parameters； 模型結構是 hyperparams

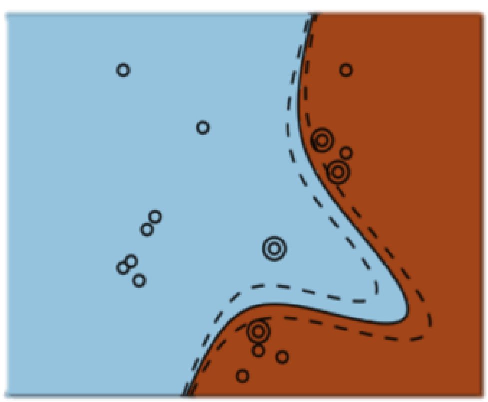


Linear Kernel



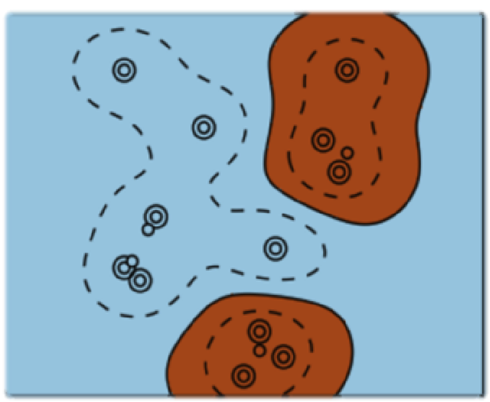
C hyperparameter

Polynomial Kernel



C plus gamma, degree and coefficient hyperparameters

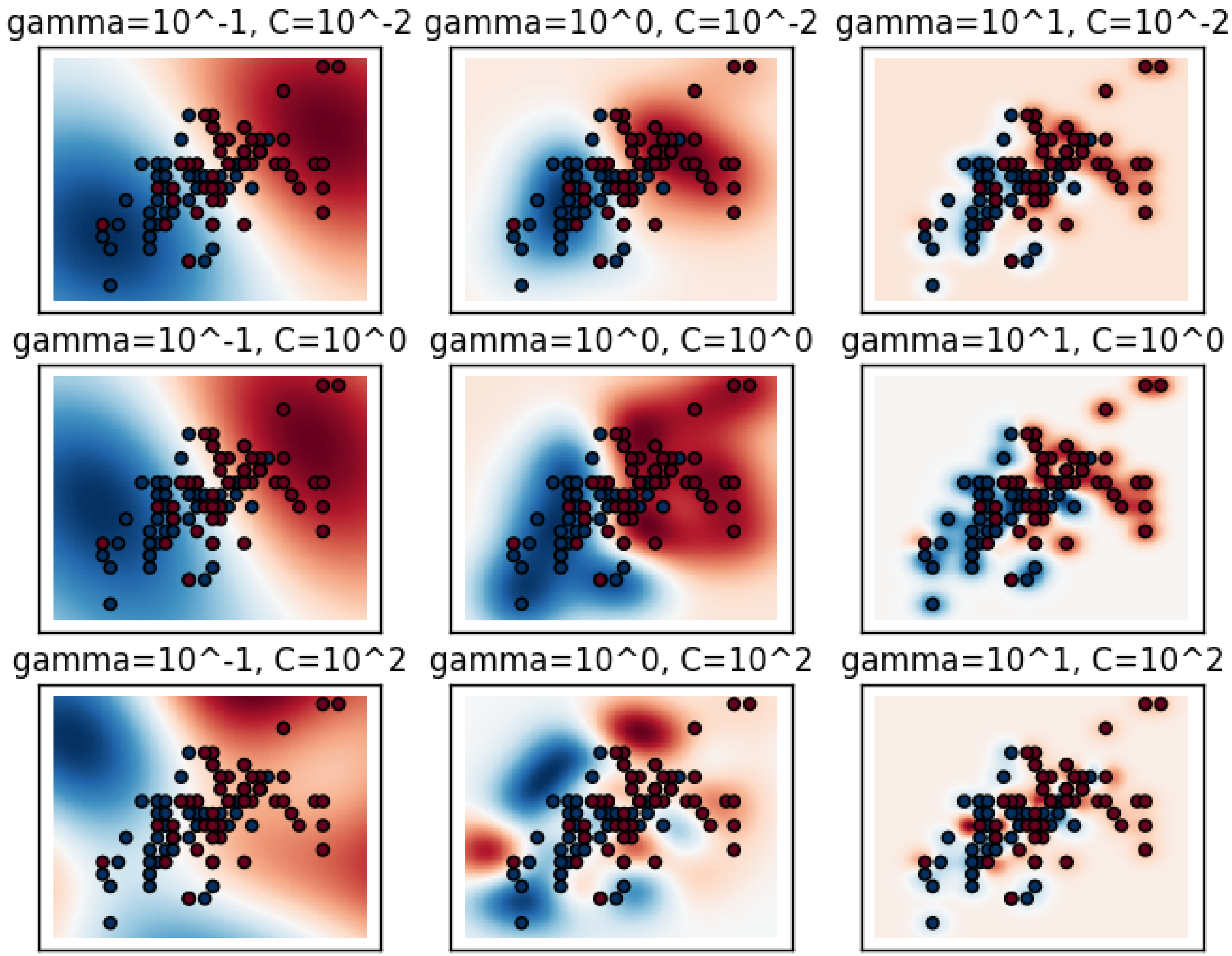
RBF Kernel



C plus gamma hyperparameter

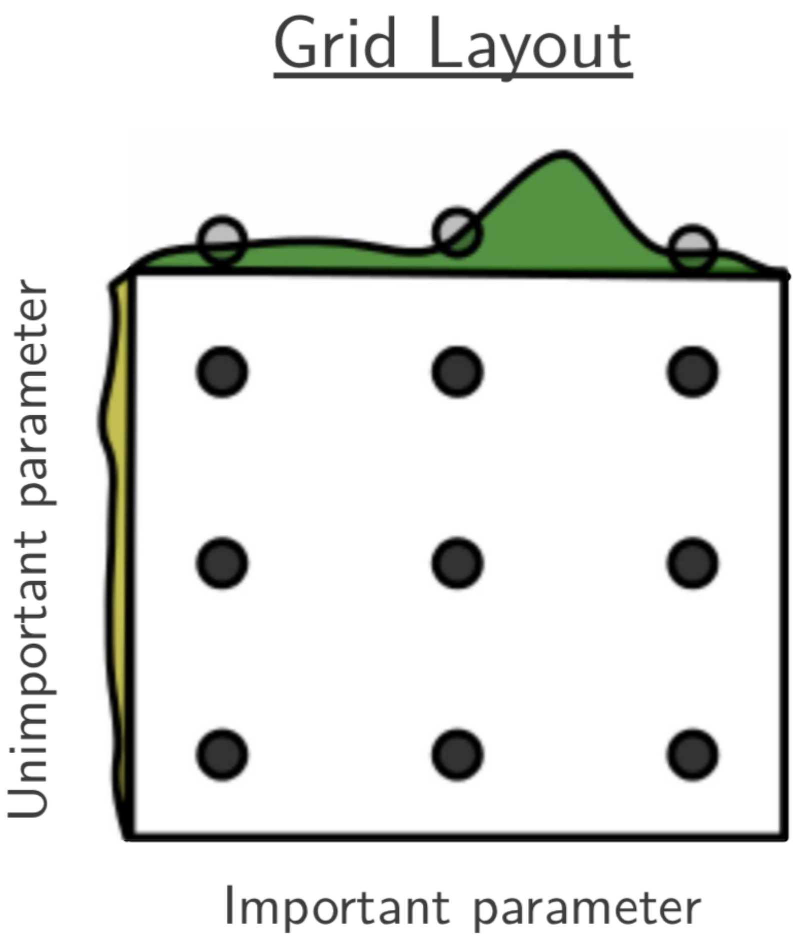
Performance Tuning: Grid Search

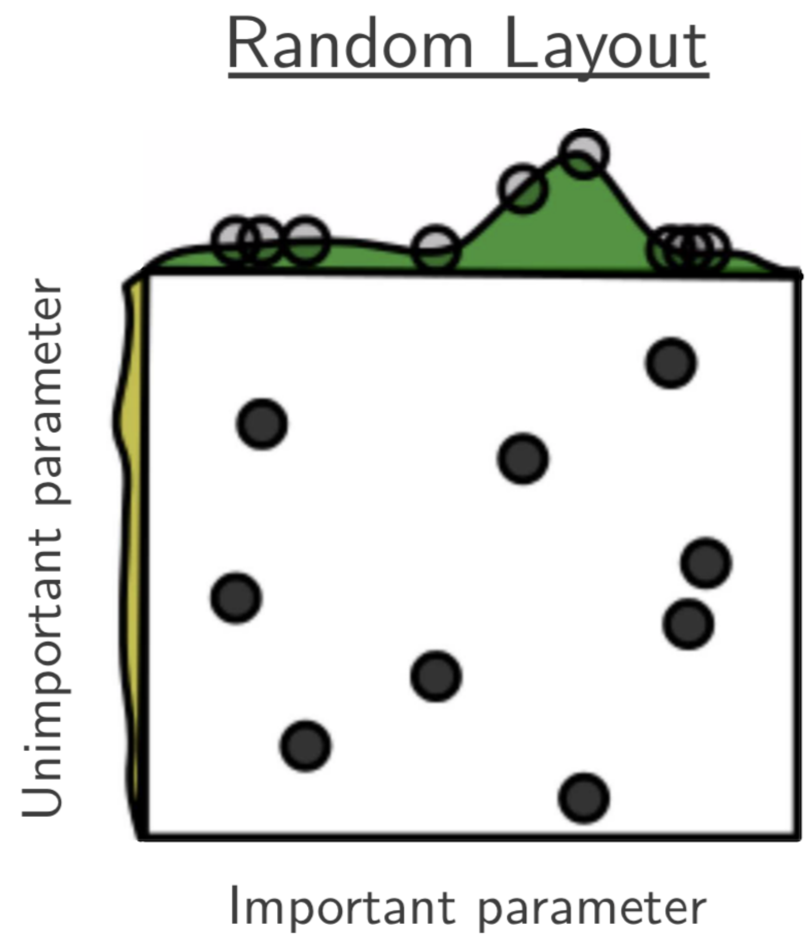
就是有系統化地改變 hyperparams 最佳化模型表現



Performance Tuning: HyperOpt

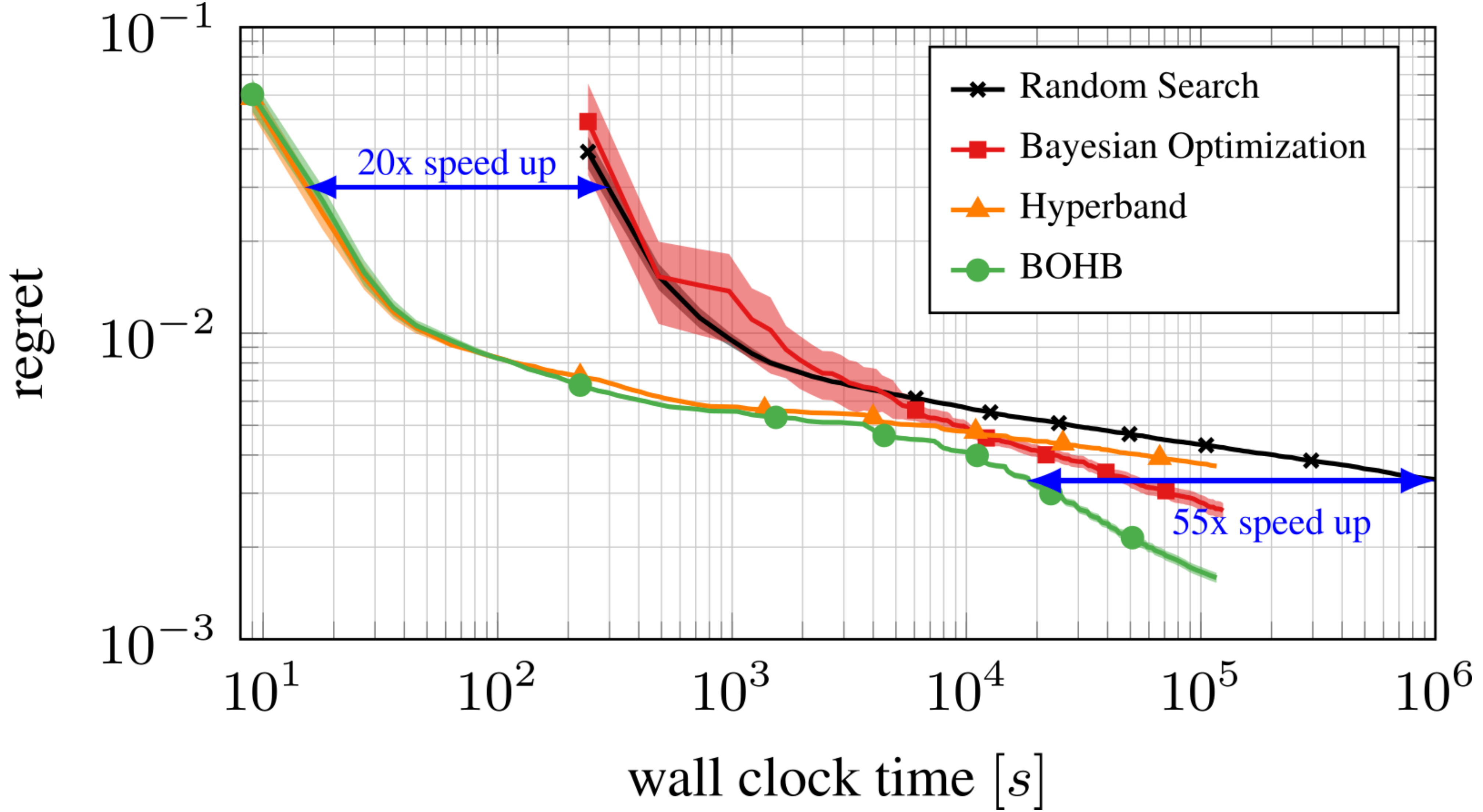
Grid Search 系統化但搜尋效率輸 Random Search





Performance Tuning: HyperBand

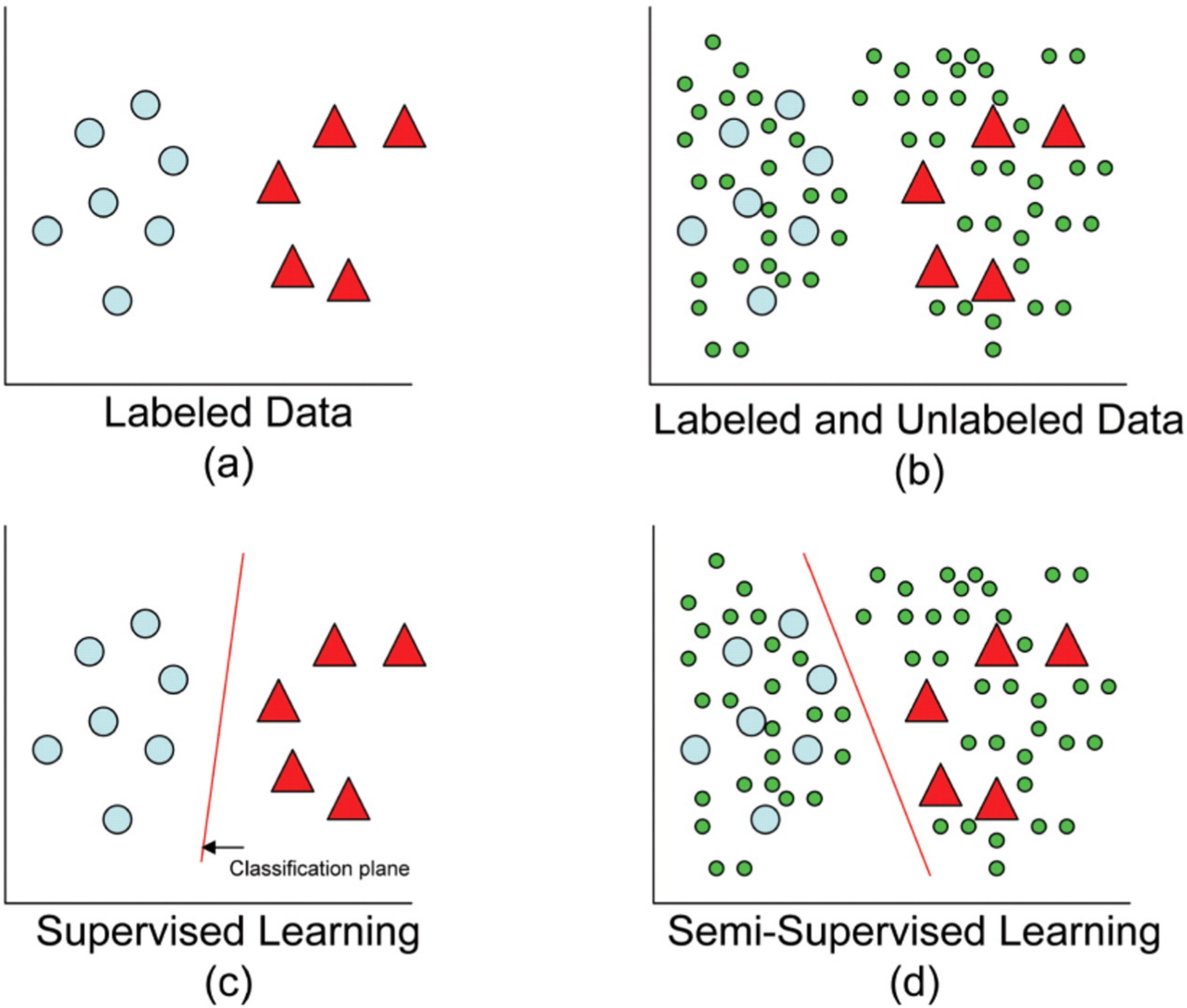
State-of-the-art: HyperBand family



半監督式學習
(Semi-supervised Learning)

Semi-supervised Learning

可利用 sklearn.semi_supervised

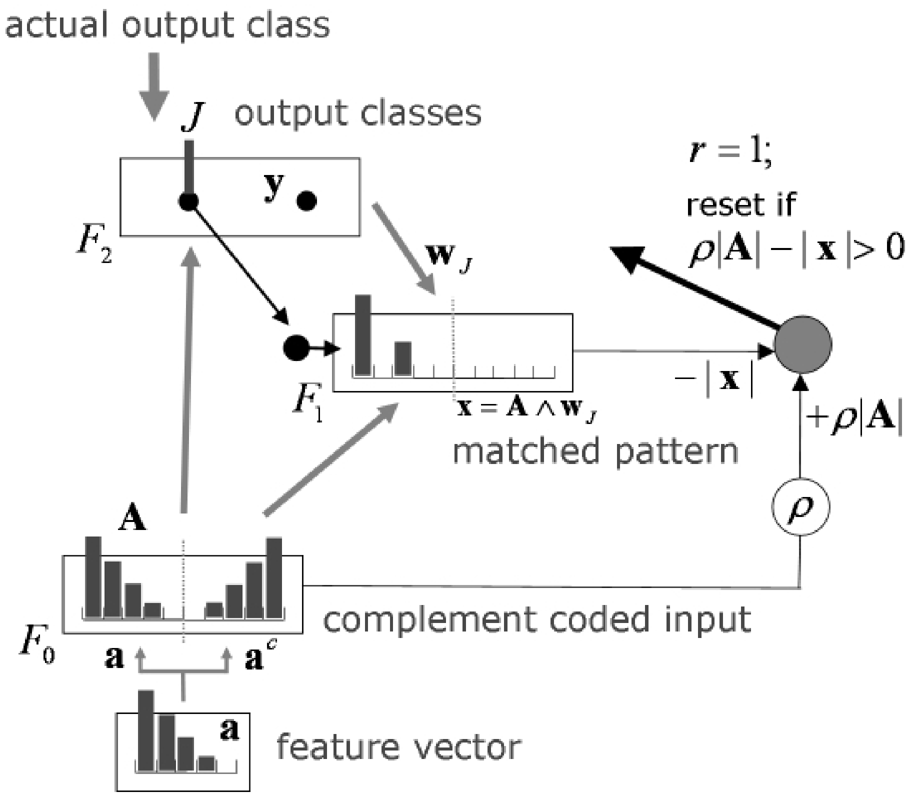


混合式學習
(Hybrid/Mixed Learning)

Hybrid Learning (1/3)

不同學習法可以混搭

如 ARTMAP中先做 unsupervised learning 再做 supervised learning:



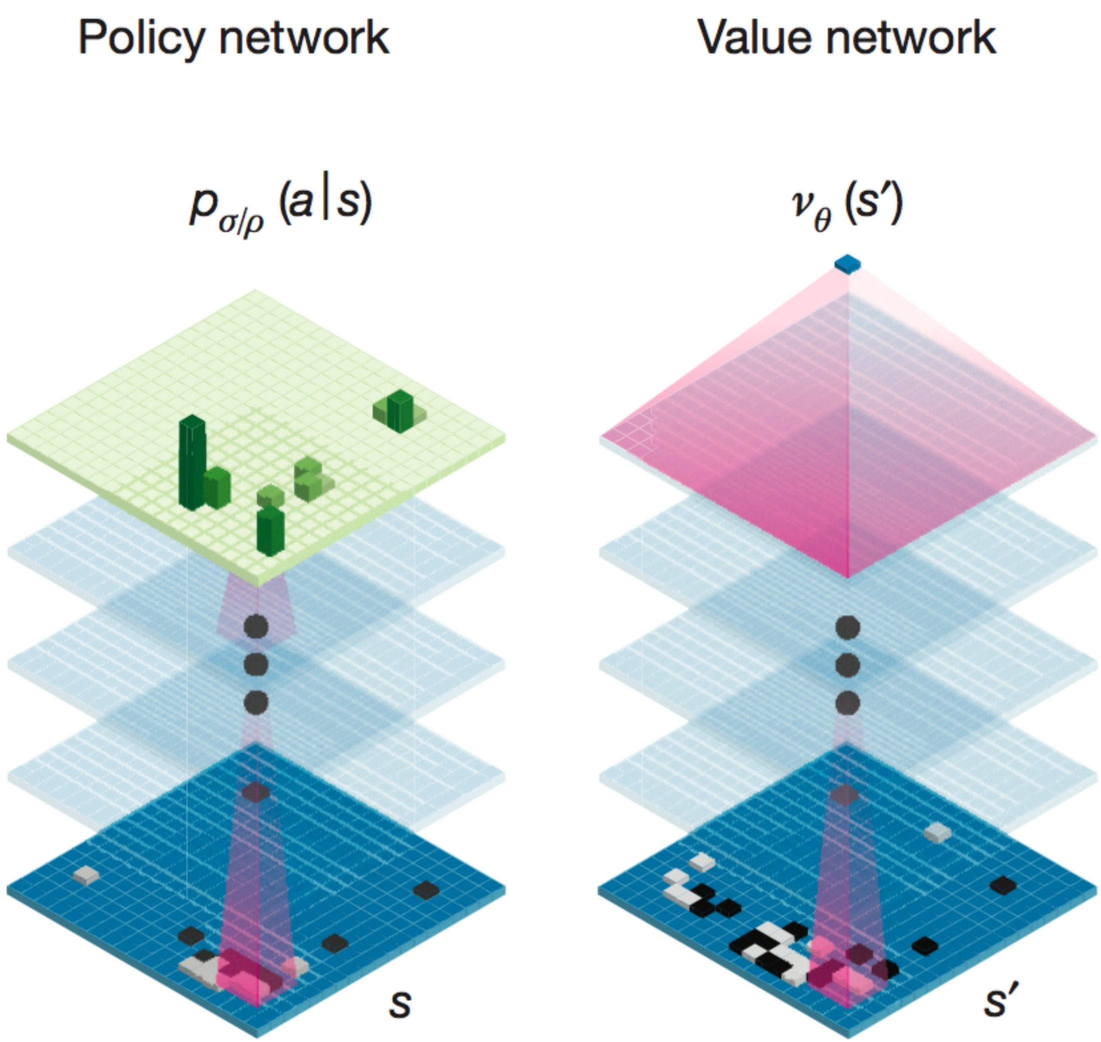
也可利用 ML 中的基因演算法去最佳化其他 ML 模型參數 :

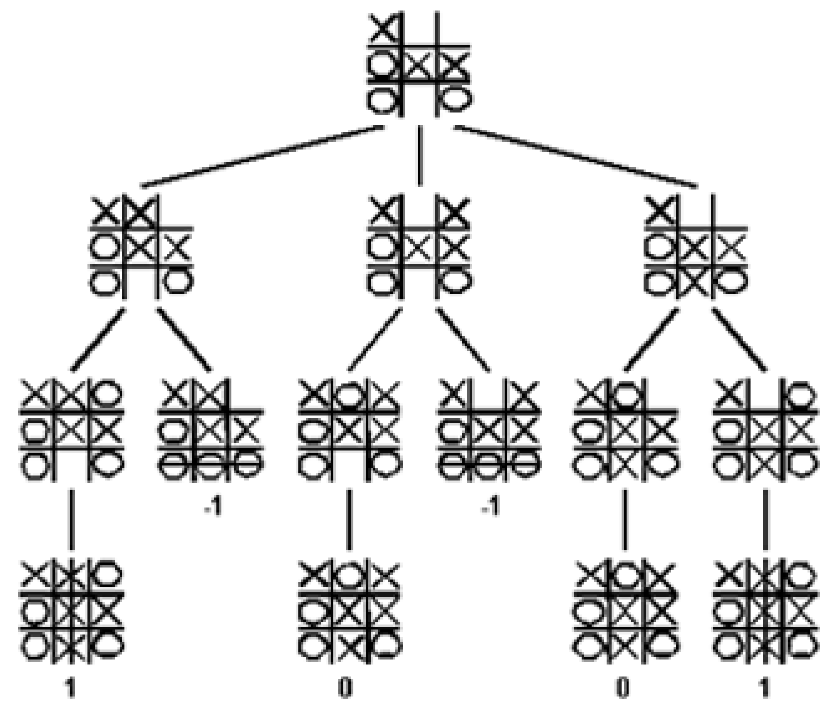
- **步驟 1**: 自行定義 fitness function y=f(***X***)
  (***X*** 為參數向量 ; f 執行模型評估 ; y 為正確率 / 錯誤率)

- **步驟 2**: 將 fitness function f 傳給基因演算法來最佳化

Hybrid Learning (2/3)

左是監督式學習；右是增強式學習





Hybrid Learning (3/3)

Neural Architecture Search with Reinforcement Learning

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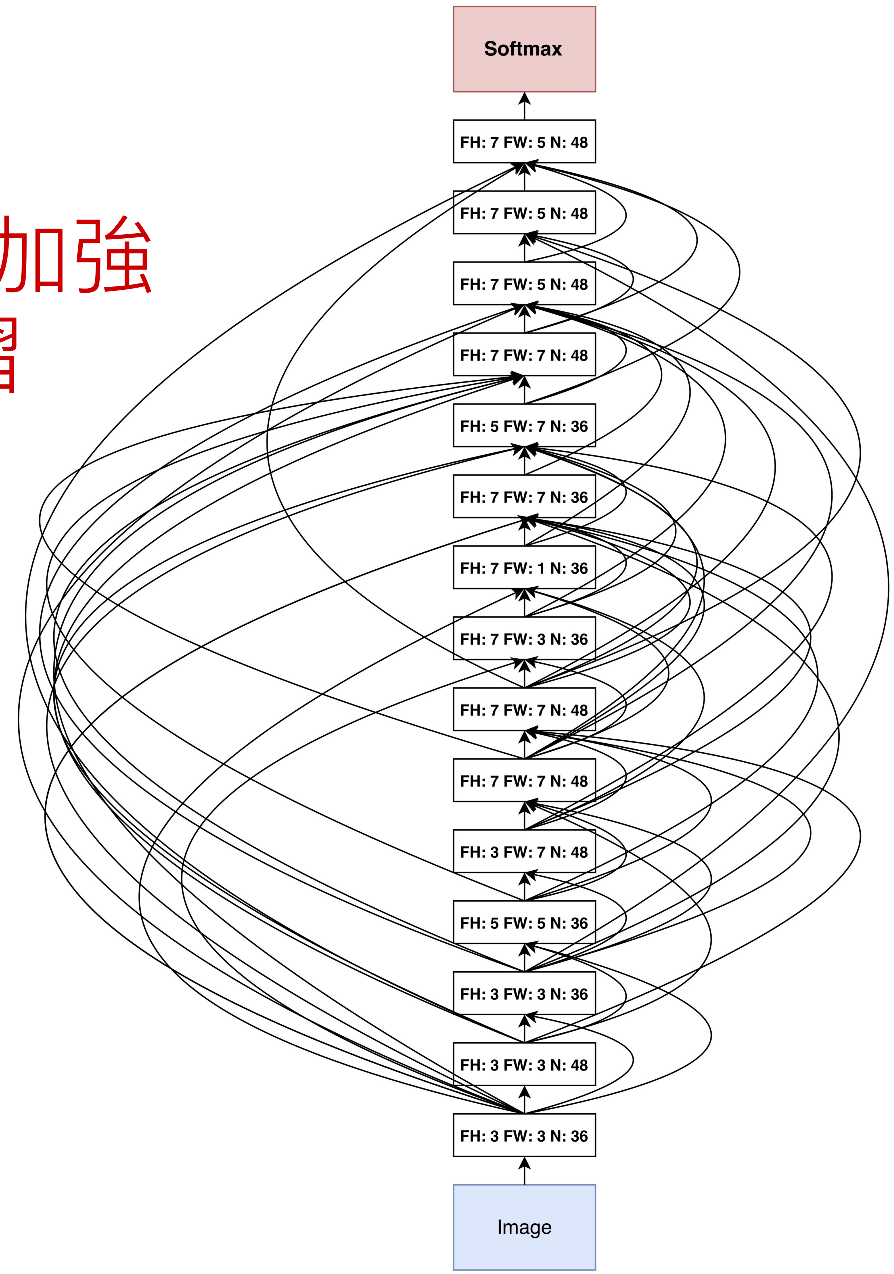
用增強式學習加強
監督式學習



Abstract

Neural networks are powerful and flexible models that work wel
cult learning tasks in image, speech and natural language unders
their success, neural networks are still hard to design. In this pa
current network to generate the model descriptions of neural ne
this RNN with reinforcement learning to maximize the expected
generated architectures on a validation set. On the CIFAR-10 data
starting from scratch, can design a novel network architecture th
human-invented architecture in terms of test set accuracy. Our (
achieves a test error rate of 3.65, which is 0.09 percent better and
the previous state-of-the-art model that used a similar architectu
the Penn Treebank dataset, our model can compose a novel recur
performs the widely-used LSTM cell, and other state-of-the-art ba
achieves a test set perplexity of 62.4 on the Penn Treebank, whic
ity better than the previous state-of-the-art model. The cell can al
to the character language modeling task on PTB and achieves
perplexity of 1.214.

Ensemble Learning

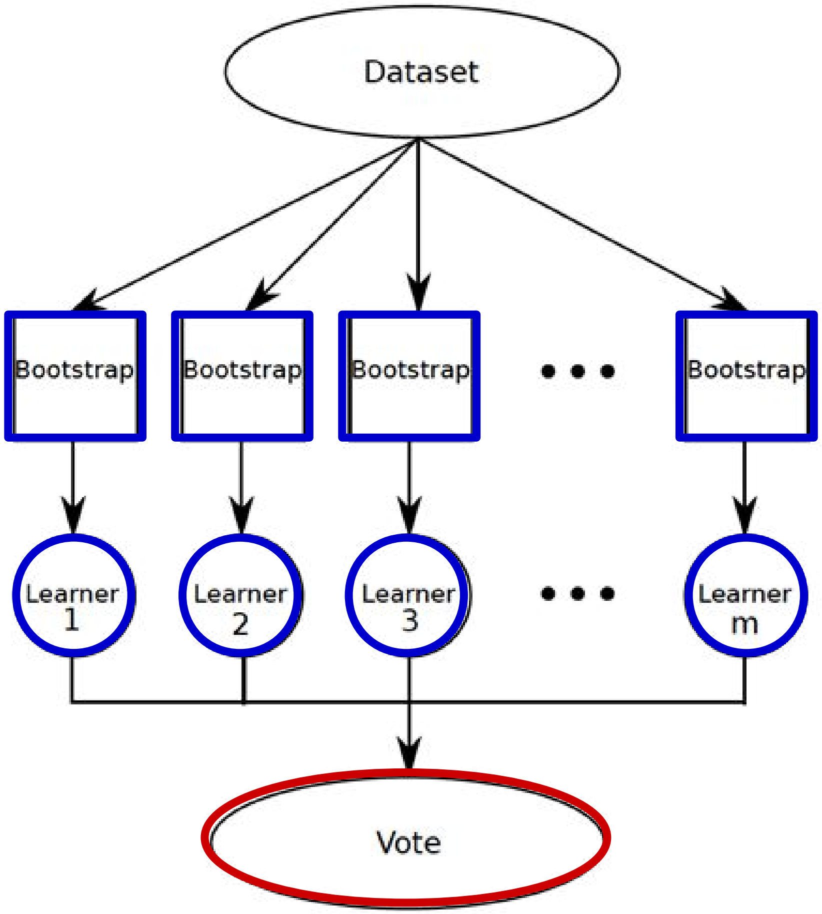
就是集結一群 machine learners 來做決策

Common Types of Ensemble Methods

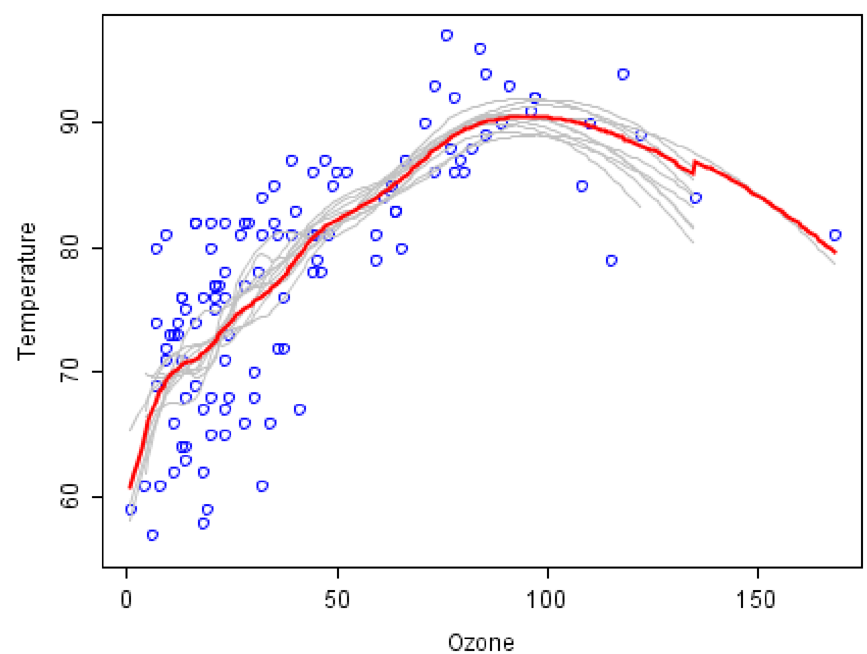
Bagging	• Reduces variance and increases accuracy • Robust against outliers or noisy data • Often used with Decision Trees (i.e. Random Forest)
Boosting	• Also reduces variance and increases accuracy • Not robust against outliers or noisy data • Flexible – can be used with any loss function
Stacking	• Used to ensemble a diverse group of strong learners • Involves training a second-level machine learning algorithm called a “metalearner” to learn the optimal combination of the base learners

Bagging

(同類的)machine learners 學不同的抽樣資料



人生的經驗不同，
做出來的判斷也不同。



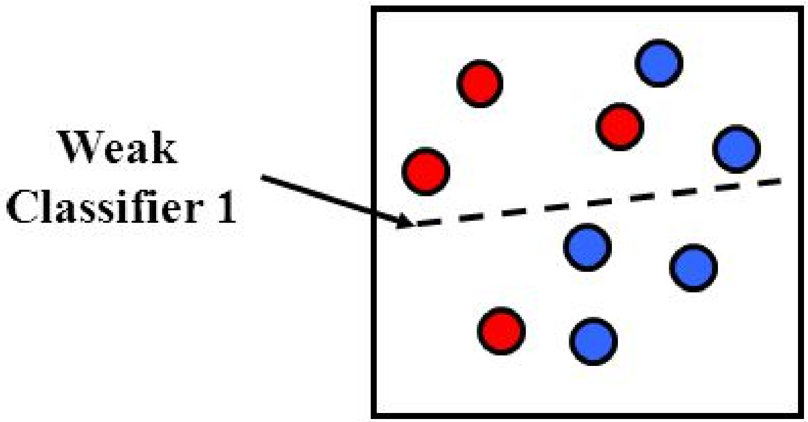
Boosting (1/3)

看起來有兩大類；但 AB 其實是 GB 的特例

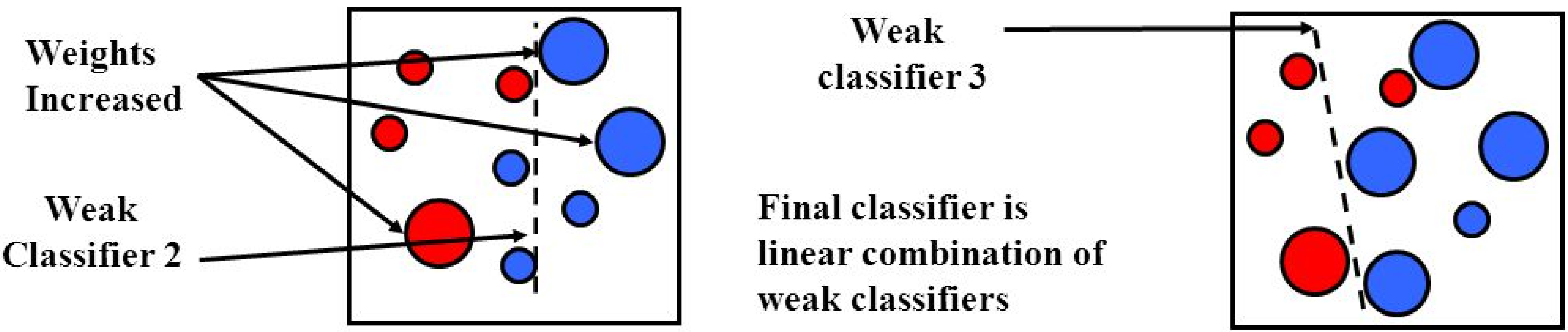
AdaBoost	GradientBoost
Both AdaBoost and Gradient Boost use a base weak learner and they try to boost the performance of a weak learner by iteratively shifting the focus towards problematic observations that were difficult to predict. At the end, a strong learner is formed by addition (or weighted addition) of the weak learners.	
In AdaBoost, shift is done by up-weighting observations that were misclassified before.	Gradient boost identifies difficult observations by large residuals computed in the previous iterations.
In AdaBoost "shortcomings" are identified by high-weight data points.	In Gradientboost "shortcomings" are identified by gradients.
Exponential loss of AdaBoost gives more weights for those samples fitted worse.	Gradient boost further dissect error components to bring in more explanation.
AdaBoost is considered as a special case of Gradient boost in terms of loss function, in which exponential losses.	Concepts of gradients are more general in nature.

Boosting (2/3): AdaBoost

Re-weighting mis-classified training data;
投票時不同 classifiers 的 weights 也不同



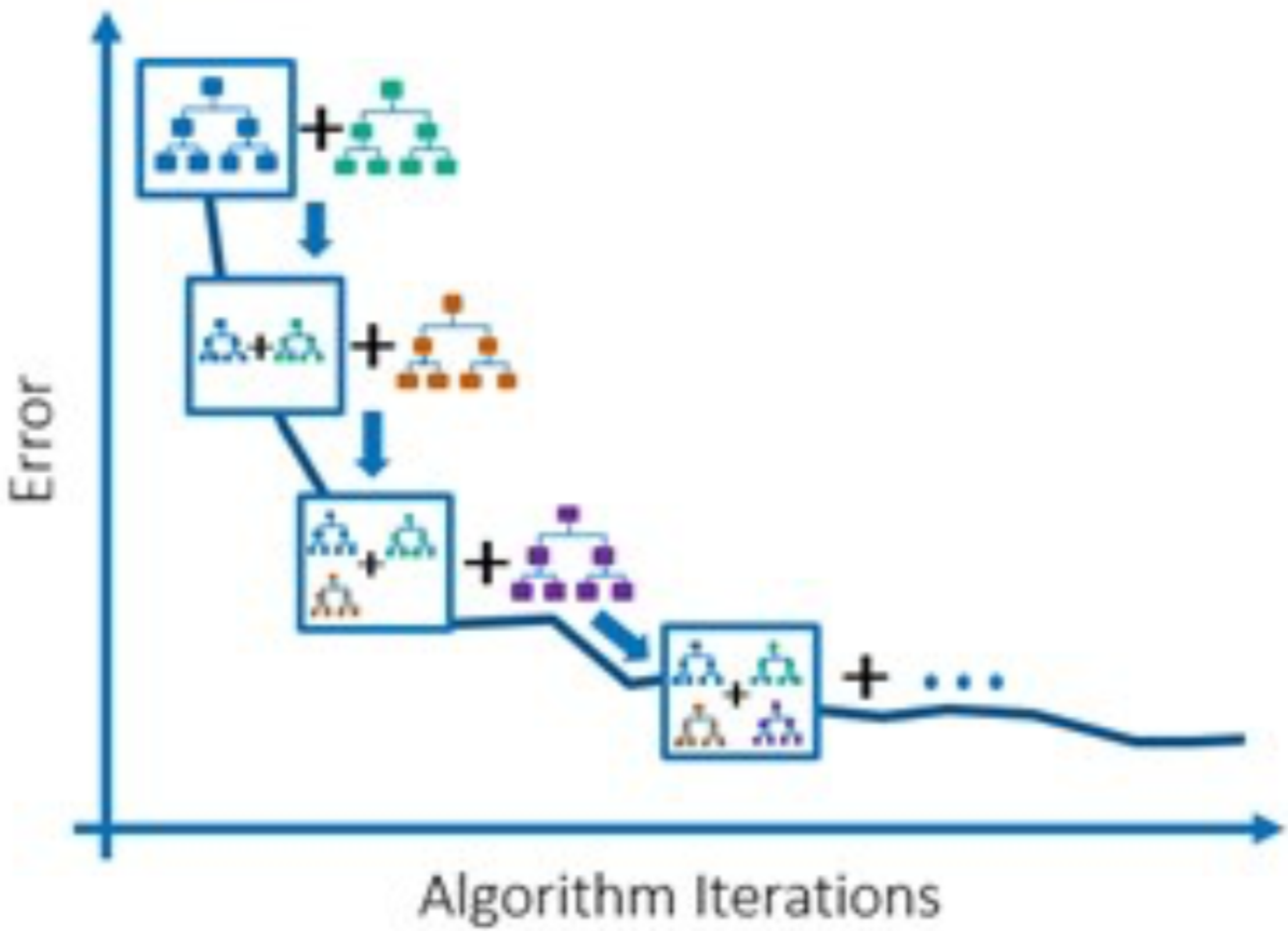
Classifier 1 學不好的繼續交給
Classifier 2 來學 / 處理 :



Boosting (3/3): GradientBoost

加入後續的 model 是為了要減少整體錯誤率

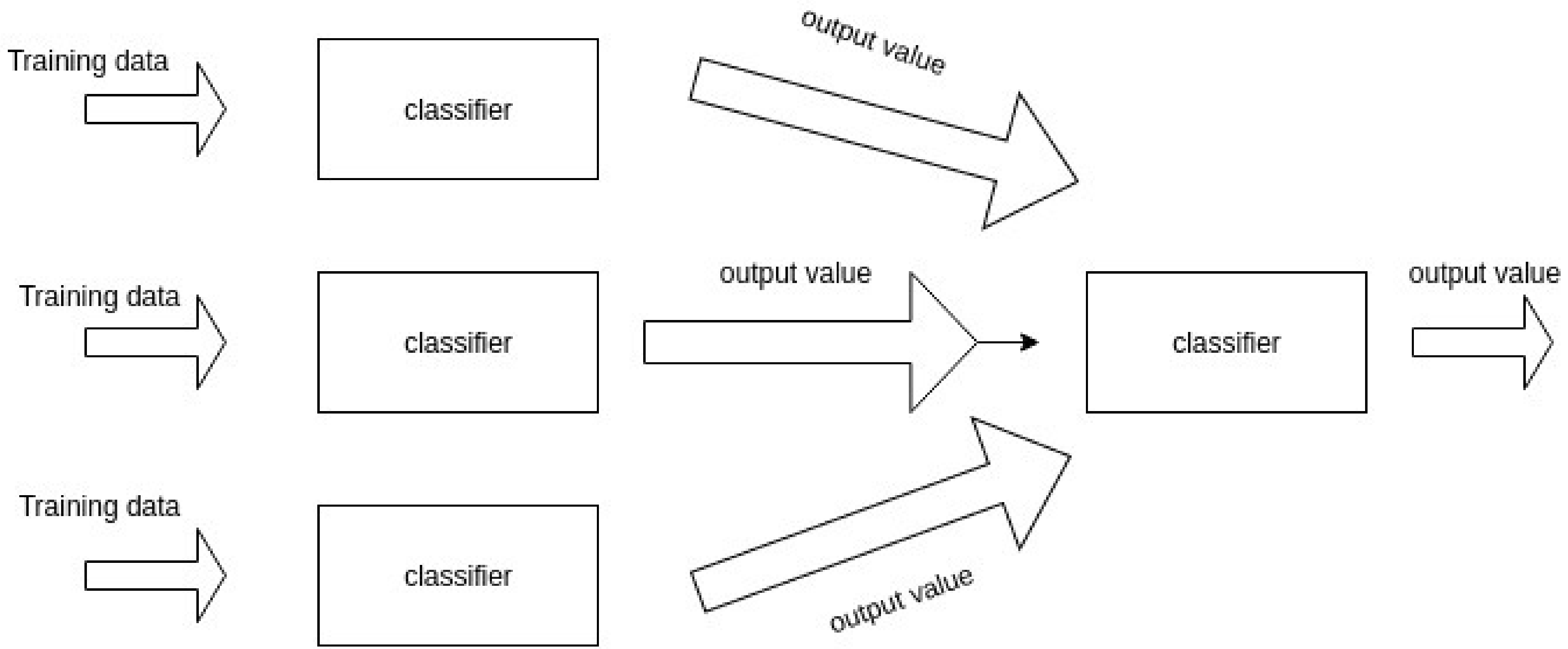
(c.f. 泰勒展開式)



流行的XGBoost是高效能的 GradientBoost 實作

Stacking

可看成 hierarchical supervised learning



雖 scikit-learn 中沒有直接支援但很容易自己實作

模型評估與選擇
(Model Selection)

Beyond Accuracy

除了正確率外還有很多模型評斷指標

		True condition			
	Total population	Condition positive	Condition negative	Prevalence $= \frac{\Sigma \text{ Condition positive}}{\Sigma \text{ Total population}}$	
Predicted condition	Predicted condition positive	**True positive**	**False positive** (Type I error)	Positive predictive value (PPV), Precision $= \frac{\Sigma \text{ True positive}}{\Sigma \text{ Test outcome positive}}$	False discovery rate (FDR) $= \frac{\Sigma \text{ False positive}}{\Sigma \text{ Test outcome positive}}$
	Predicted condition negative	**False negative** (Type II error)	**True negative**	False omission rate (FOR) $= \frac{\Sigma \text{ False negative}}{\Sigma \text{ Test outcome negative}}$	Negative predictive value (NPV) $= \frac{\Sigma \text{ True negative}}{\Sigma \text{ Test outcome negative}}$
	Accuracy (ACC) = $\frac{\Sigma \text{ True positive} + \Sigma \text{ True negative}}{\Sigma \text{ Total population}}$	True positive rate (TPR), Sensitivity, Recall $= \frac{\Sigma \text{ True positive}}{\Sigma \text{ Condition positive}}$	False positive rate (FPR), Fall-out $= \frac{\Sigma \text{ False positive}}{\Sigma \text{ Condition negative}}$	Positive likelihood ratio (LR+) $= \frac{\text{TPR}}{\text{FPR}}$	Diagnostic odds ratio (DOR) $= \frac{\text{LR+}}{\text{LR–}}$
		False negative rate (FNR), Miss rate $= \frac{\Sigma \text{ False negative}}{\Sigma \text{ Condition positive}}$	True negative rate (TNR), Specificity (SPC) $= \frac{\Sigma \text{ True negative}}{\Sigma \text{ Condition negative}}$	Negative likelihood ratio (LR–) $= \frac{\text{FNR}}{\text{TNR}}$	

Precision = 提取出的正確信息數 / 提取出的信息數

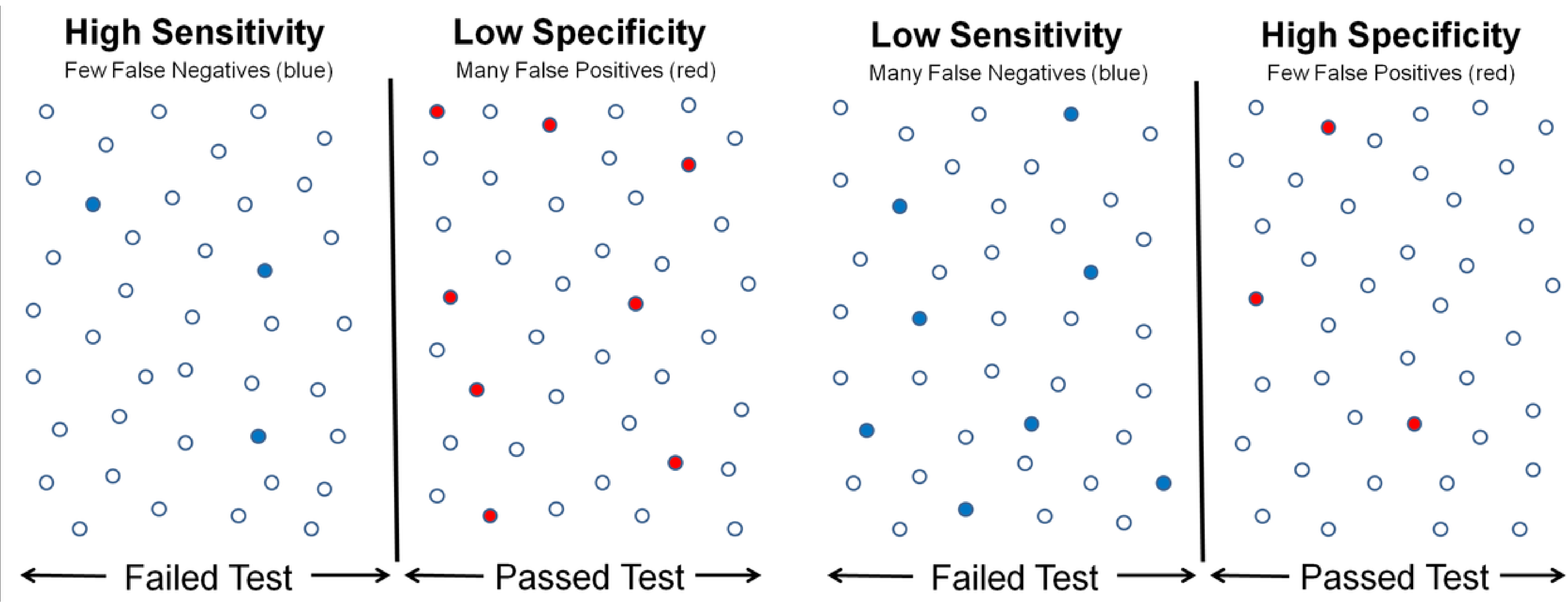
Recall = 提取出的正確信息數 / 樣本的正確信息數

F1= 兩者的調和平均 =2*Precision*Recall/(Precision+Recall)

G= 兩者的幾何平均 =sqrt(Precision*Recall)

Sensitivity vs. Specificity

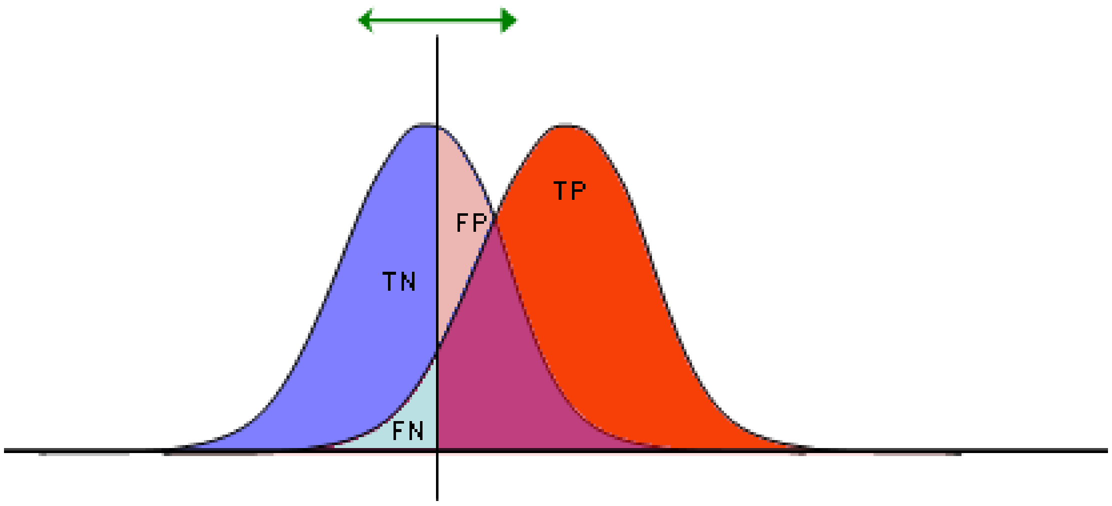
Sensitivity = 預測有 / 真的有
Specificity = 預測沒有 / 真的沒有



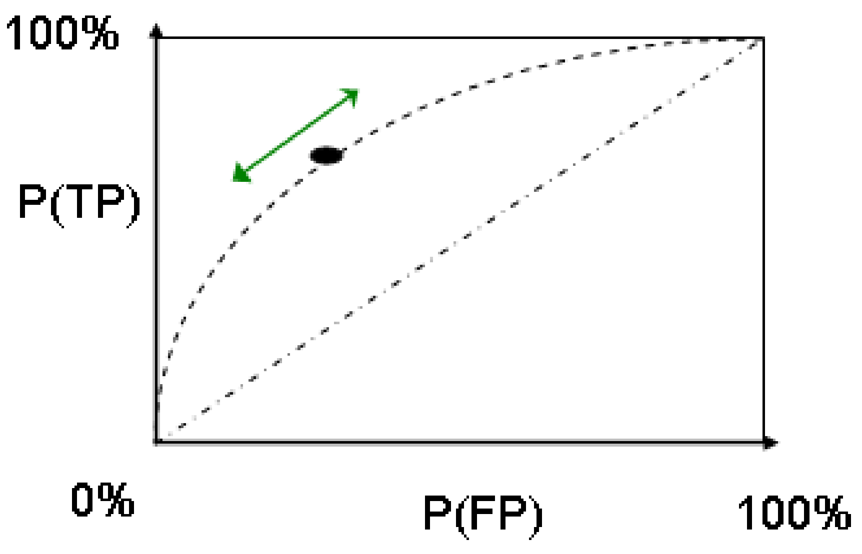
Sensitivity 和 Specificity 是一個 trade-off

ROC Curves (1/2)

改變 decision boundary 就會改變 sensitivity 與 specificity 的比例

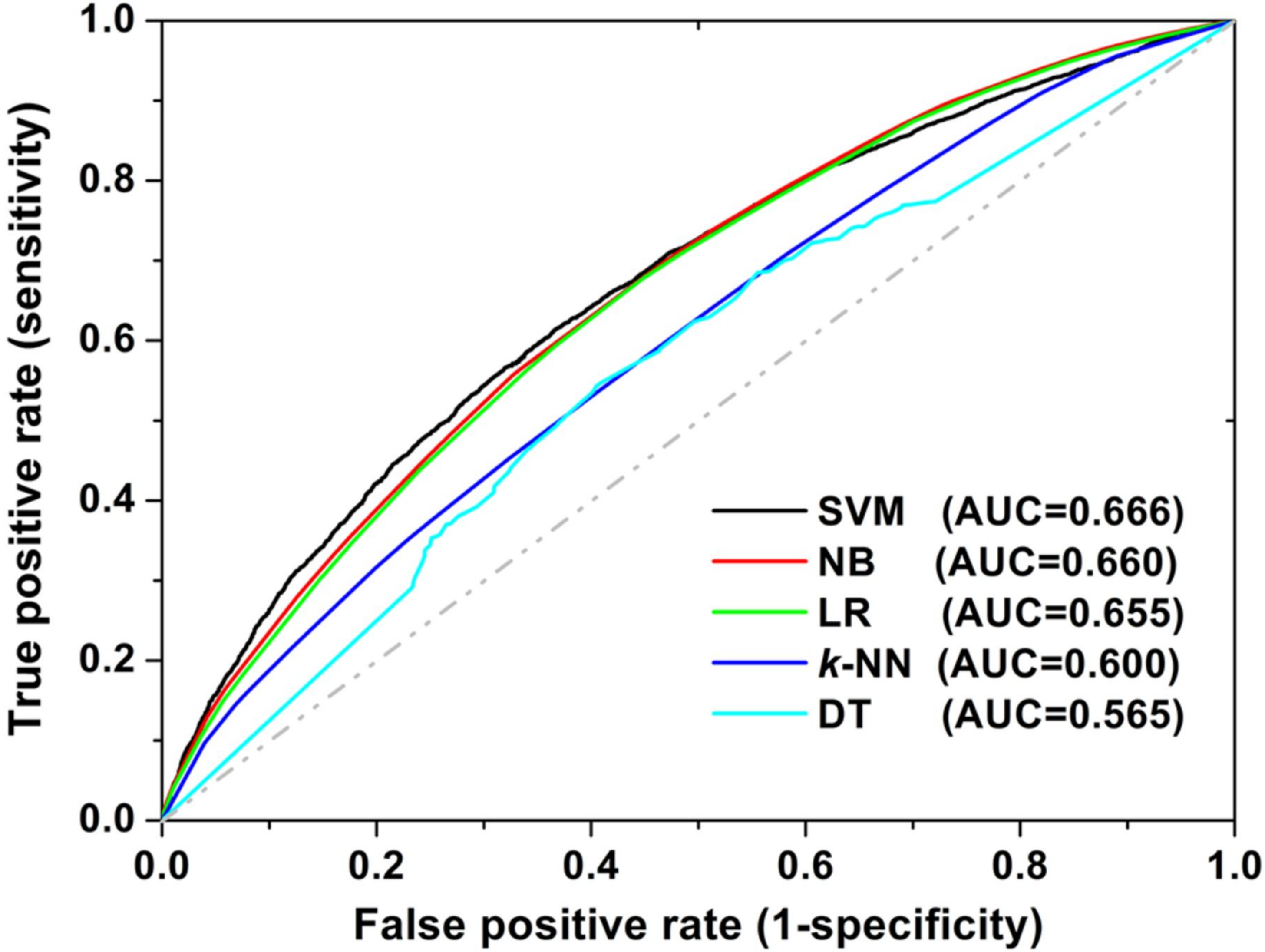


TP	FP
FN	TN
1	1



ROC Curves (2/2)

目標在找出 Area Under Curve 最大的線
也就是 sensitivity 和 specificity 同時最好的方法



Game Over