### **Introduction to Machine Learning**

DBDA.X408.(33)

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#### Week 5

Decision Tree.

Boosting.

Support Vector Machines.

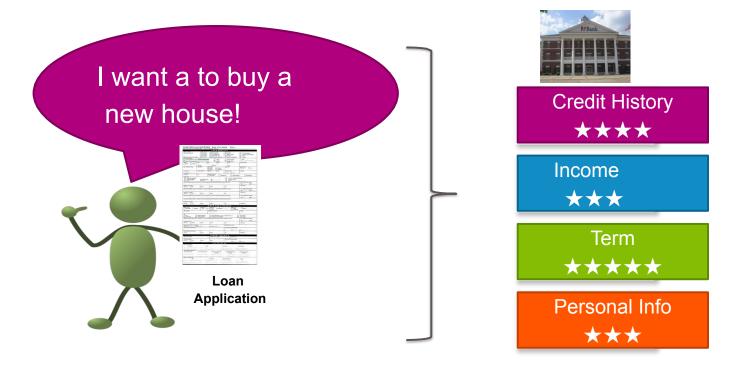
Colab Demonstration.



## **Decision Tree**



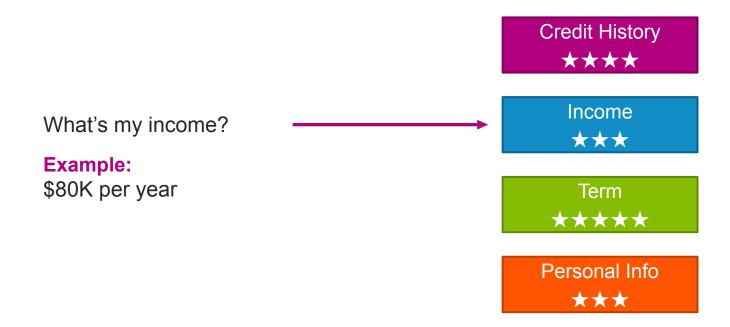
### What makes a loan risky?



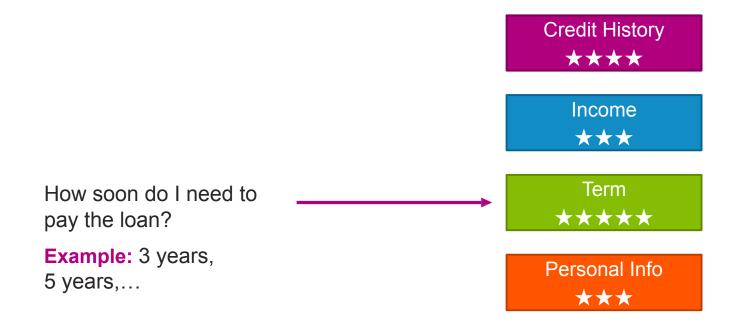


**Credit History** Did I pay previous loans \*\*\* on time? **Example:** excellent, good, Income or fair \*\*\* Term \*\*\*\* Personal Info \*\*\*



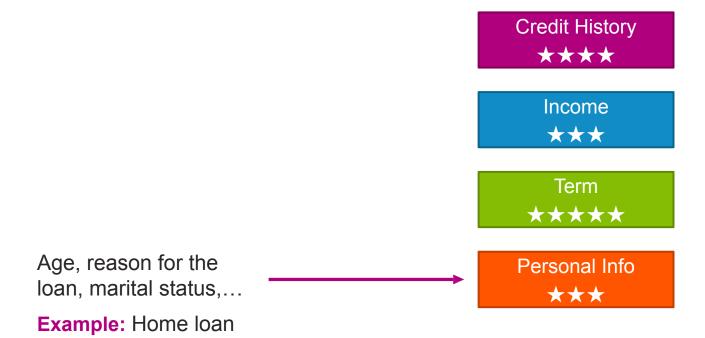








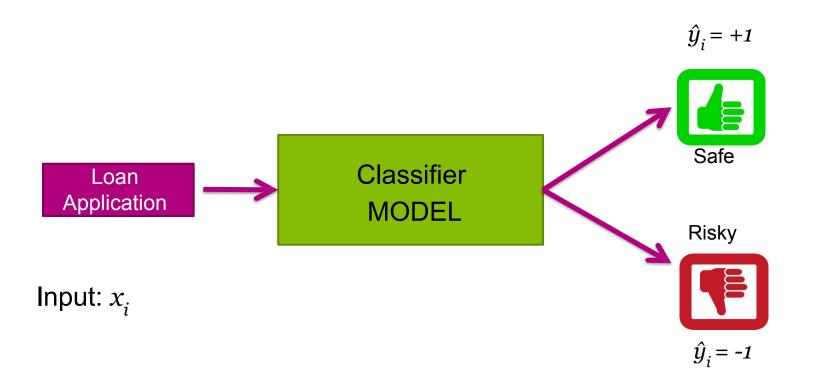
for a married couple



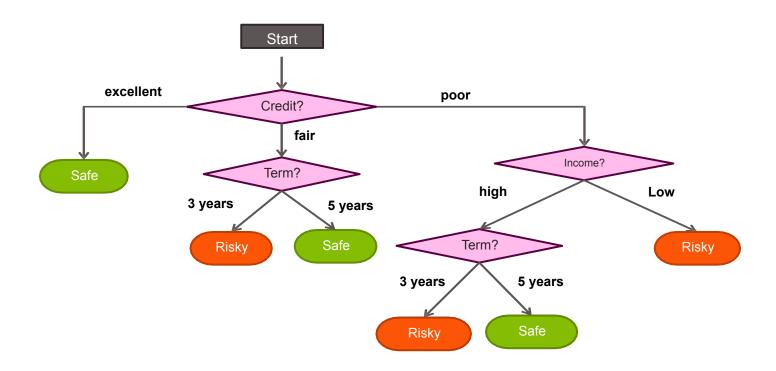


#### Classifier Review

#### Output: $\hat{y}$ Predicted class



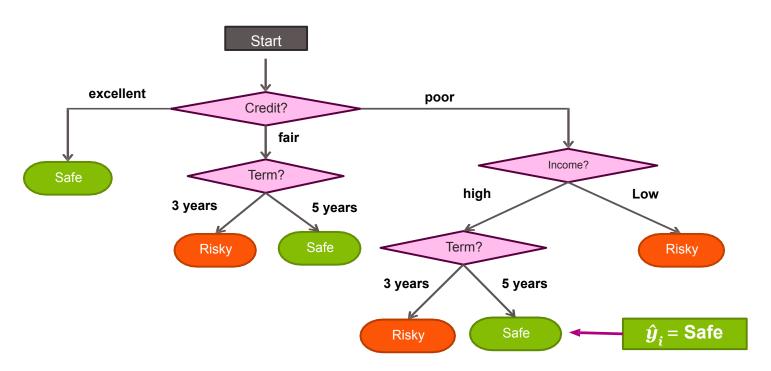
#### **Decision Tree**





#### **Decision Tree**

 $x_i = (Credit = poor, Income = high, Term = 5 years)$ 



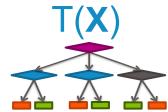


### Decision Tree Learning Problem

Training data: N observations  $(x_i, y_i)$ 

Credit	Term	Income	у
excellent	3 yrs	high	safe
fair	5 yrs	low	risky
fair	3 yrs	high	safe
poor	5 yrs	high	risky
excellent	3 yrs	low	risky
fair	5 yrs	low	safe
poor	3 yrs	high	risky
poor	5 yrs	low	safe
fair	3 yrs	high	safe





### Quality Metric: Classification error

Error measures fraction of mistakes:

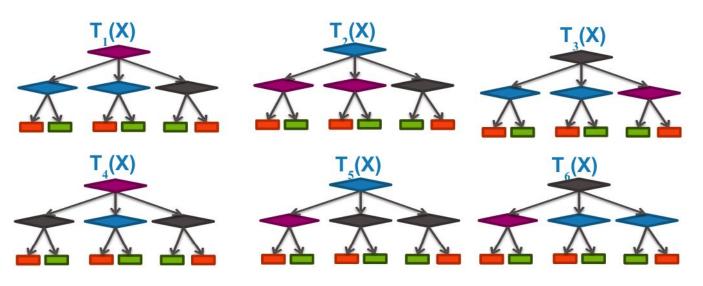
Error = # incorrect predictions / # example

- Best possible value : 0.0
- Worst possible value: 1.0



#### How do we find the best tree?

Exponentially large number of possible trees makes decision tree learning hard!



Learning the smallest decision tree is an *NP-hard problem* [Hyafil & Rivest '76]

# **Greedy Decision Tree Learning**

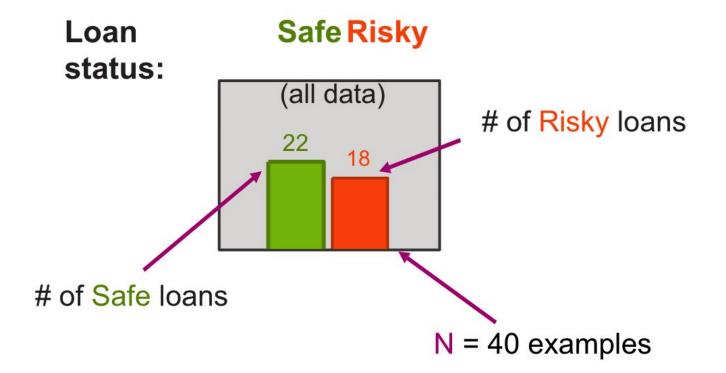


### Our Training Data Table

#### Assume N = 40, 3 features

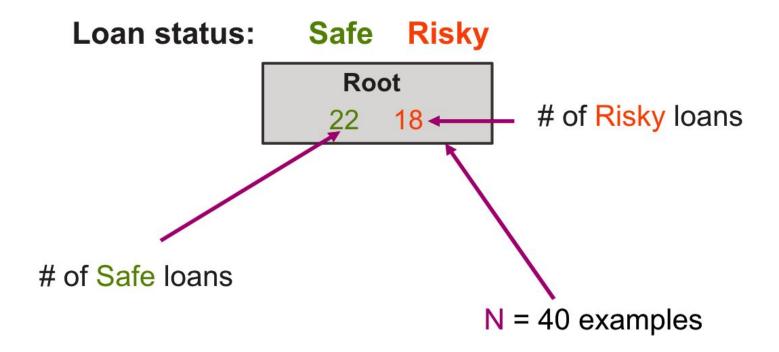
Credit	Term	Income	У
excellent	3 yrs	high	safe
fair	5 yrs	low	risky
fair	3 yrs	high	safe
poor	5 yrs	high	risky
excellent	3 yrs	low	risky
fair	5 yrs	low	safe
poor	3 yrs	high	risky
poor	5 yrs	low	safe
fair	3 yrs	high	safe

#### Start With All The Data



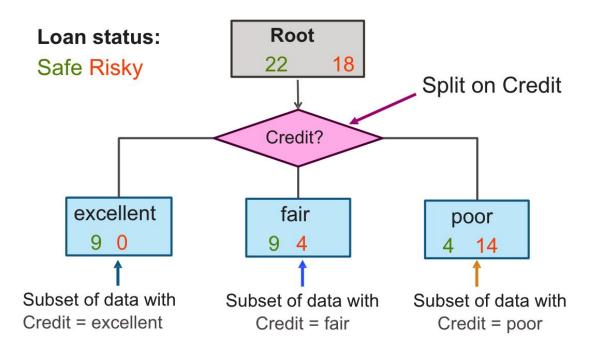


#### Compact Visual Notation: Root Node



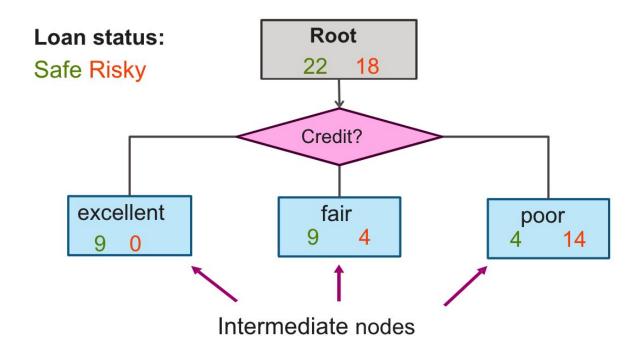


#### Decision Stump: Single Level Lree

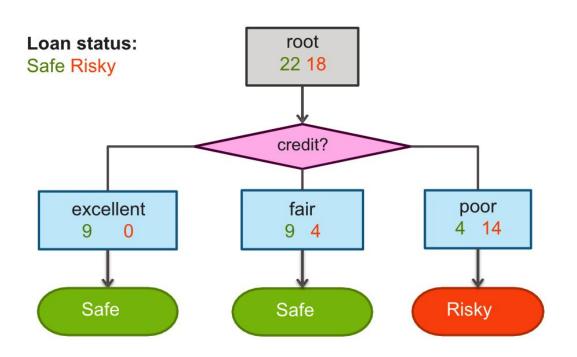




#### Visual Notation: Intermediate Nodes



### Making Predictions With a Decision Stump



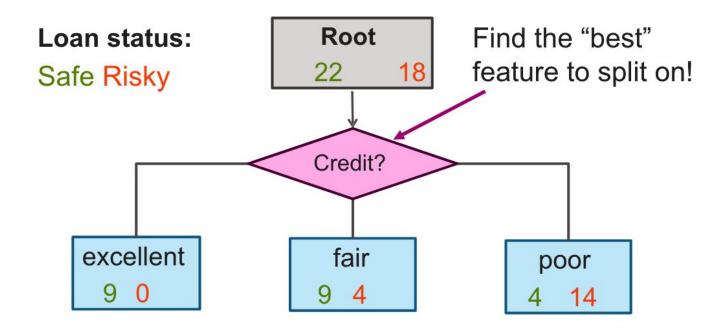
For each intermediate node, set  $\hat{y}$  = majority value



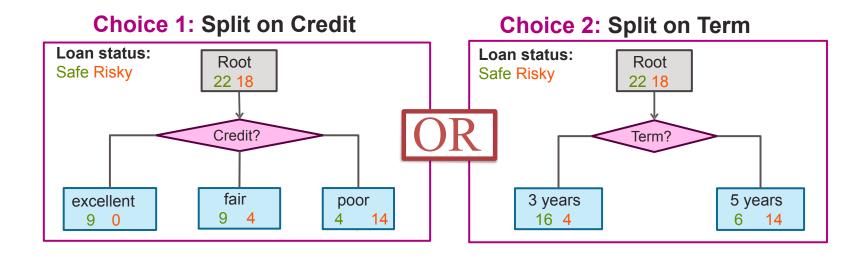
## Selecting The Best Feature To Split On



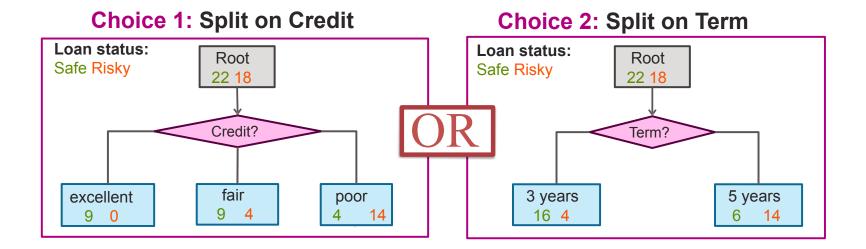
### How do we learn a decision stump?



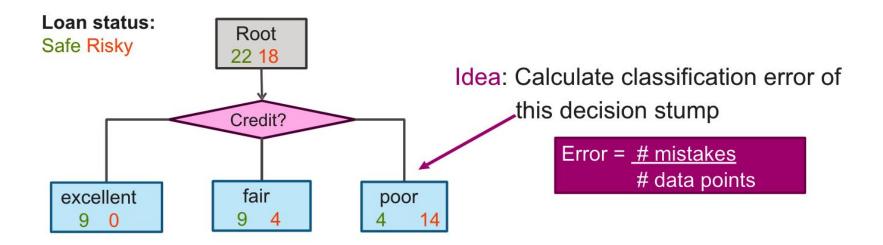
#### How do we select the best feature?



#### How do we select the best feature?



#### How do we measure effectiveness of a split?

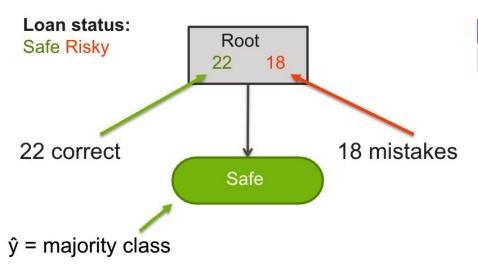




### Calculating Classification Error

Step 1:  $\hat{y}$  = class of majority of data in node

Step 2: Calculate classification error of predicting  $\hat{y}$  for this data

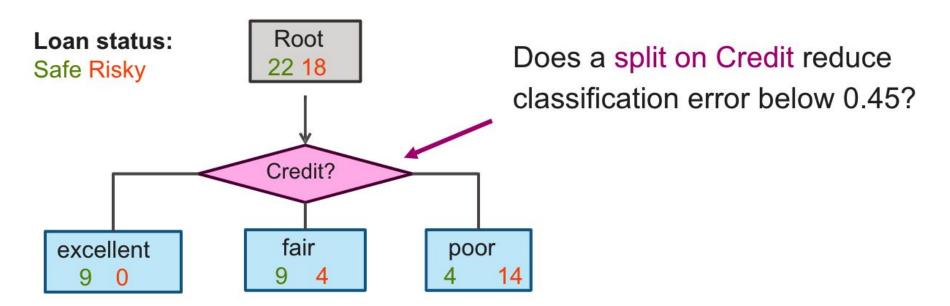


Tree	Classification error
(root)	0.45

How to do the calculation?

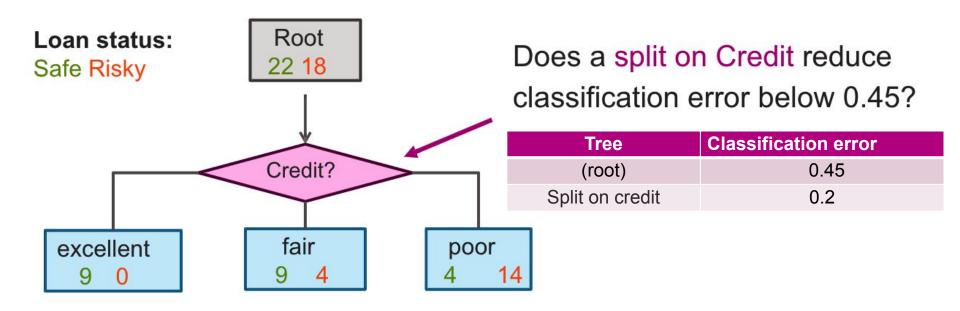


### Choice 1: Split on Credit history?



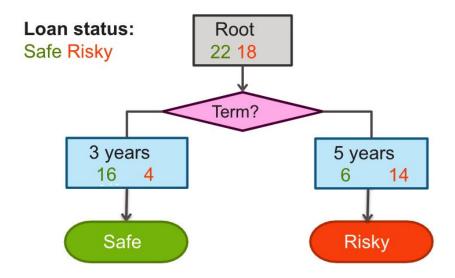


#### Choice 1: Split on Credit history?



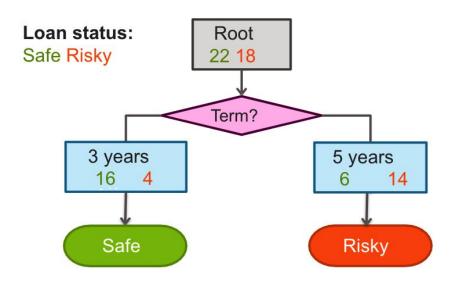


### Choice 2: Split on Term?





### Choice 2: Split on Term?



Tree	Classification error
(root)	0.45
Split on credit	0.2
Split on term	0.25



#### Choice 1 or Choice 2?

Tree	Classification error
(root)	0.45
Split on credit	0.2
Split on term	0.25

## **Choice 1: Split on Credit**

**Choice 2: Split on Term** Loan status: Loan status: Root Root Safe Risky Safe Risky 22 18 22 18 Credit? Term? fair excellent poor 3 years 5 years 14 16 4 14

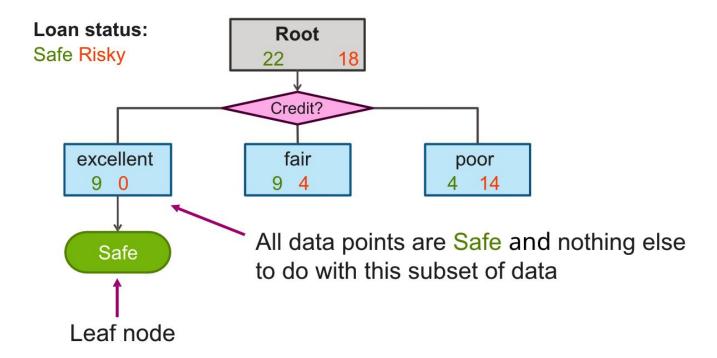
### Feature Split Selection Algorithm

- Given a subset of data M (a node in a tree)
- For each feature  $h_i(x)$ :
  - 1. Split data of M according to feature  $h_i(x)$
  - 2. Compute classification error of split
- Chose feature  $h^*(x)$  with lowest classification error

## Recursion & Stopping conditions

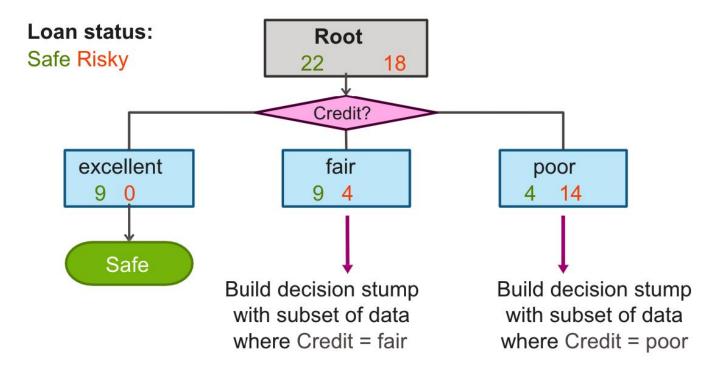


### Can We Reuse The Data After Split?



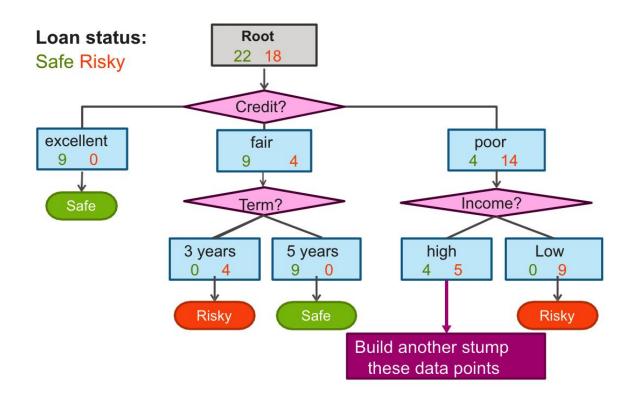


### Tree Learning = Recursive Stump Learning



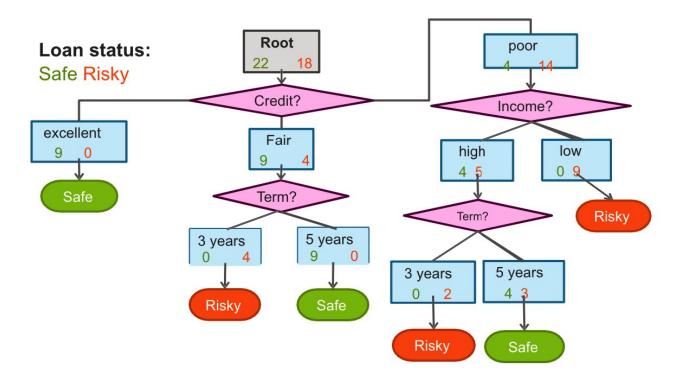


#### Second Level





#### **Final Decision Tree**

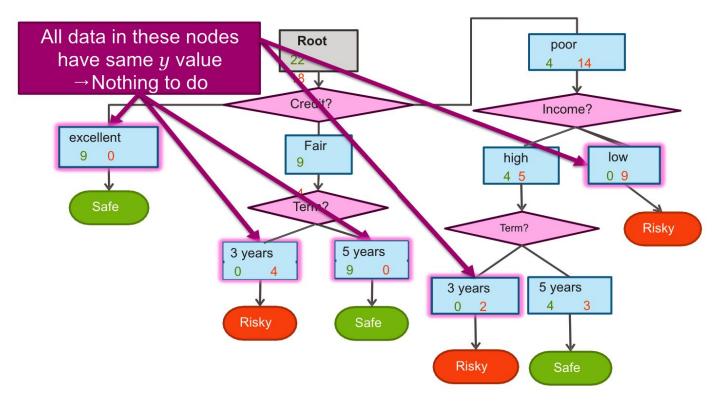


#### Simple greedy decision tree learning

Pick best feature to split on Learn decision stump with this split For each leaf of decision stump, recurse When do we stop???

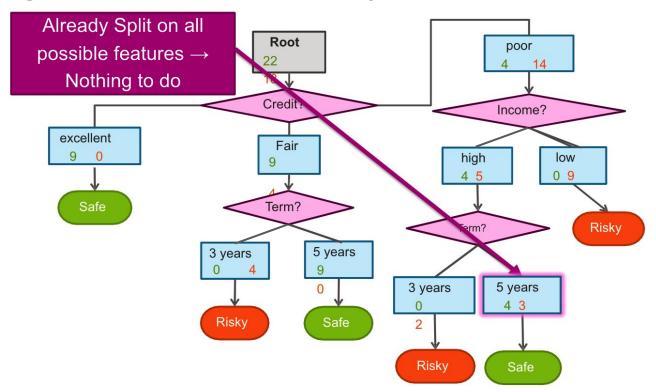


#### Stopping Condition 1: All Data Agrees On y





#### Stopping Condition 2: Already Split On All Features





#### Greedy Decision Tree Learning

• Step 1: Start with an empty tree

Step 2: Select a feature to split data

For each split of the tree:

 Step 3: If nothing more to do, make predictions

 Step 4: Otherwise, go to Step 2 & continue (recurse) on this split Pick feature split leading to lowest classification error

Stopping conditions

Recursion



#### Is This a Good Idea?





# Stopping condition 3: Don't stop if error doesn't decrease???

 $\boldsymbol{y} = \boldsymbol{x}_{[1]} \operatorname{xor} \boldsymbol{x}_{[2]}$ 

<b>x</b> [1]	<b>x</b> [2]	y
False	False	False
False	True	True
True	False	True
True	True	False

y values
True False

Root 2 2

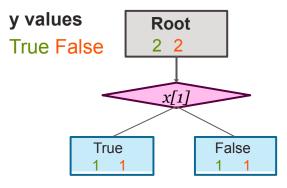
Tree	Classification error
(root)	0.5



# Consider Split On $x_{[1]}$

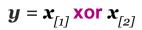
$$\boldsymbol{y} = \boldsymbol{x}_{[1]} \operatorname{xor} \boldsymbol{x}_{[2]}$$

<b>x</b> [1]	<b>x</b> [2]	y
False	False	False
False	True	True
True	False	True
True	True	False



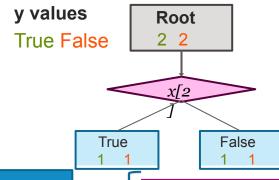
Tree	Classification error
(root)	0.5
Split on x[1]	0.5

# Consider Split On $x_{[2]}$



<b>x</b> [1]	<b>x</b> [2]	y
False	False	False
False	True	True
True	False	True
True	True	False

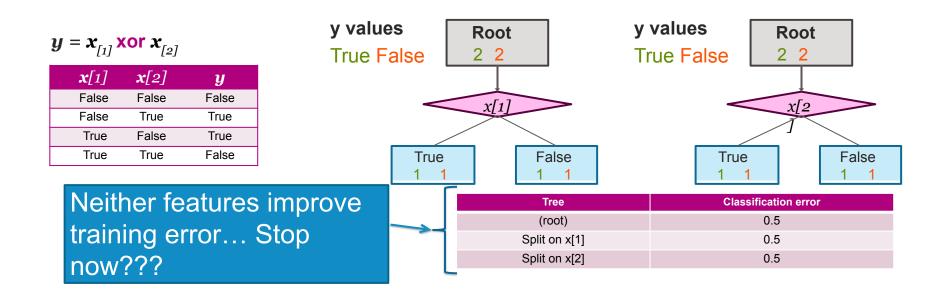
Neither features improve training error... Stop now???



Tree	Classification error
(root)	0.5
Split on x[1]	0.5
Split on x[2]	0.5

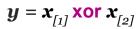


# Consider Split On $x_{[2]}$

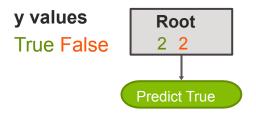




### Final Tree With Stopping Condition 3



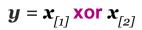
<b>x</b> [1]	<b>x</b> [2]	y
False	False	False
False	True	True
True	False	True
True	True	False



Tree	Classification error
with stopping condition 3	0.5

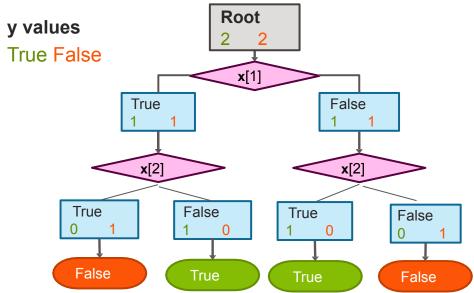
#### Without Stopping Condition 3

#### Condition 3 (stopping when training error doesn't' improve) is not recommended!



<b>x</b> [1]	<b>x</b> [2]	y
False	False	False
False	True	True
True	False	True
True	True	False

Tree	Classification error
with stopping condition 3	0.5
without stopping condition 3	



# Decision Tree Learning: Real Valued Features

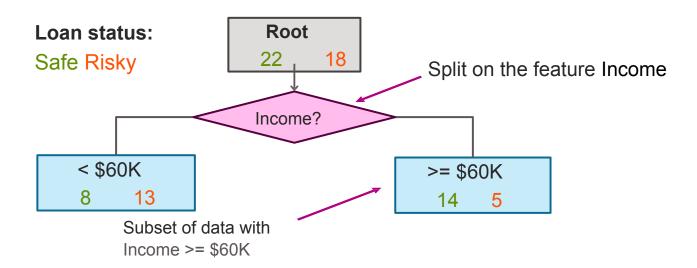


#### How Do We Use Real Values Inputs?

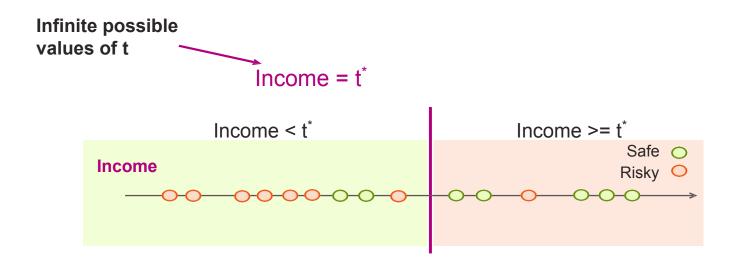
Income	Credit	Term	У
\$105 K	excellent	3 yrs	Safe
\$112 K	good	5 yrs	Risky
\$73 K	fair	3 yrs	Safe
\$69 K	excellent	5 yrs	Safe
\$217 K	excellent	3 yrs	Risky
\$120 K	good	5 yrs	Safe
\$64 K	fair	3 yrs	Risky
\$340 K	excellent	5 yrs	Safe
\$60 K	good	3 yrs	Risky



#### Threshold Split

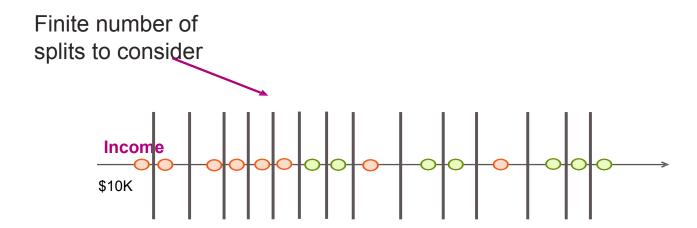


#### Finding The Best Threshold Split





#### Only Need To Consider Mid-points

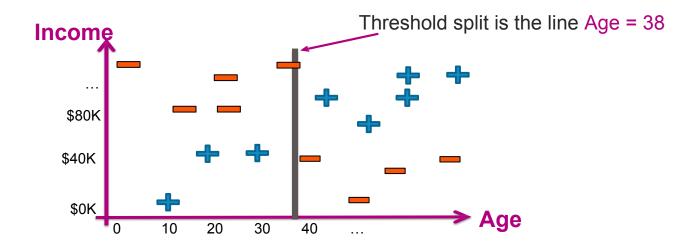




#### Threshold split selection algorithm

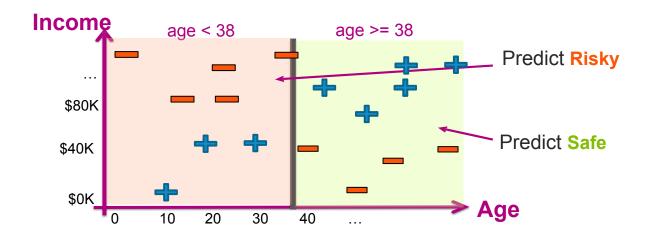
- Step 1: Sort the values of a feature  $h_j(x)$ : Let  $\{v_1, v_2, v_3, \dots v_N\}$  denote sorted values
- Step 2:
  - For i = 1 ... N-1
    - Consider split  $t_i = (v_i + v_{i+1})/2$
    - Compute classification error for threshold split  $h_i(x) >= t_i$
  - Chose the t\* with the lowest classification error

## Visualizing the threshold split

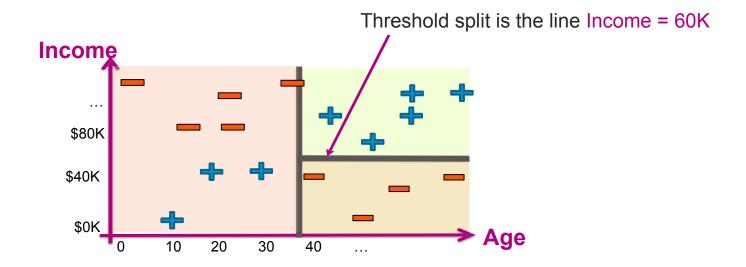




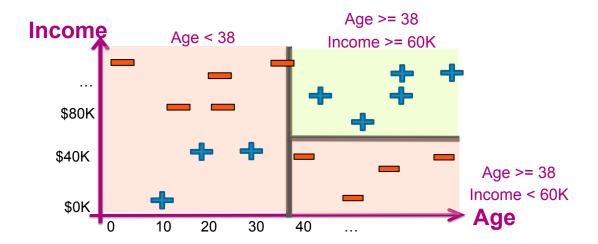
## Split on Age >= 38



## Depth 2: Split on Income >= \$60K



#### Each split partitions the 2-D space

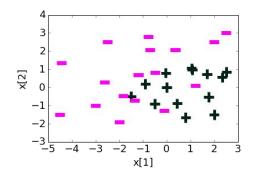


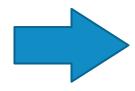
# Decision trees vs logistic regression: Example

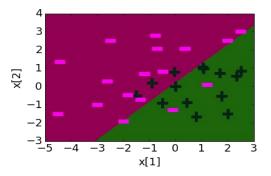


## Logistic Regression

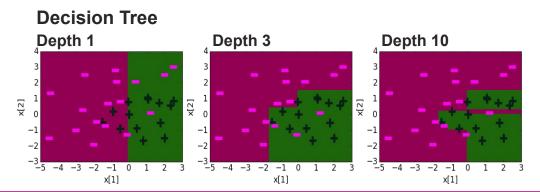
Feature	Value	Weight Learned
$h_o(x)$	1	0.22
$h_{i}(x)$	x[1]	1.12
$h_2(x)$	x[2]	-1.07



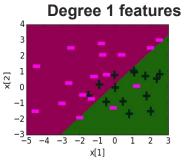


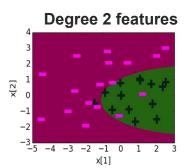


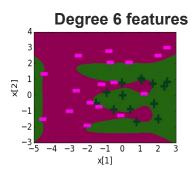
#### Comparing decision boundaries













#### What you can do now

- Define a decision tree classifier
- Interpret the output of a decision trees
- Learn a decision tree classifier using greedy algorithm
- Traverse a decision tree to make predictions
  - Majority class predictions
- Tackle continuous and discrete features



# Boosting



#### Simple (Weak) Classifiers Are Good

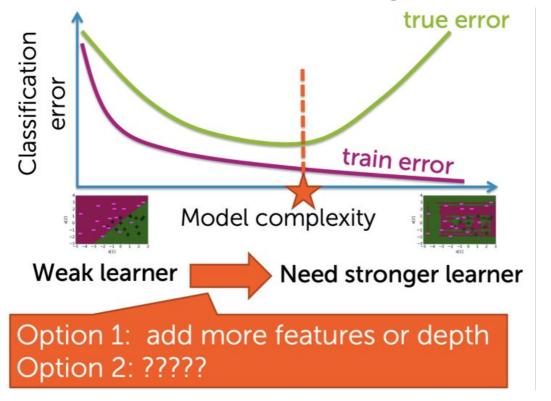


Low variance. Learning is fast!

But high bias...



#### FInding A Classifier That's Just Right





#### Boosting

"Can a set of weak learners be combined to create a stronger learner?" *Kearns and Valiant (1988)* 



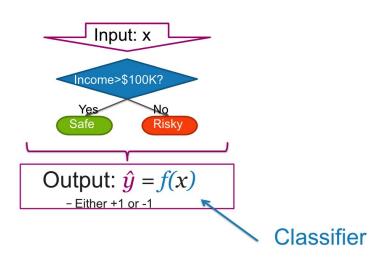




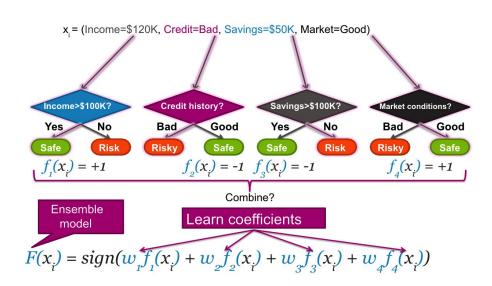
Amazing impact: • simple approach • widely used in industry • wins most Kaggle competitions • great systems (e.g., XGBoost)



#### **Ensemble Classifier**



A single classifier



Ensemble methods: Each classifier "votes" on prediction



#### **Ensemble Classifier in General**

- Goal:
  - Predict output y
    - Either +1 or -1
  - From input x
- Learn ensemble model:
  - Classifiers:  $f_1(x), f_2(x), ..., f_T(x)$
  - Coefficients:  $\hat{w}_{_{1}}$ ,  $\hat{w}_{_{2}}$ , ...,  $\hat{w}_{_{T}}$
- Prediction:

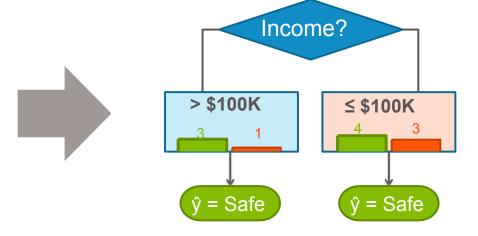
$$\hat{y} = sign\left(\sum_{t=1}^{T} \hat{\mathbf{w}}_t f_t(\mathbf{x})\right)$$

### Training a Classifier

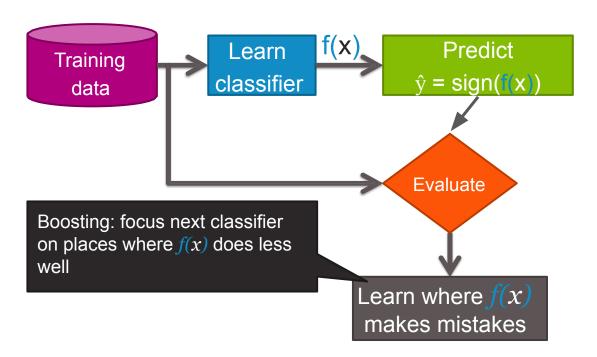


## Learning Decision Stump

Credit	Income	у
Α	\$130K	Safe
В	\$80K	Risky
С	\$110K	Risky
А	\$110K	Safe
А	\$90K	Safe
В	\$120K	Safe
С	\$30K	Risky
С	\$60K	Risky
В	\$95K	Safe
А	\$60K	Safe
А	\$98K	Safe



#### Boosting = Focus Learning on "Hard" Points





## Learning on Weighted Data:

More weight on "hard" or more important points

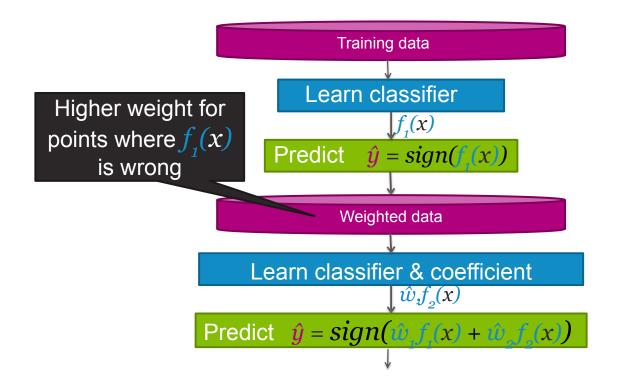
- Weighted dataset:
  - Each  $x_i$ ,  $y_i$  weighted by  $\alpha_i$ 
    - More important point = higher weight  $\alpha_i$
- Learning:
  - Data point *i* counts as  $\alpha_i$  data points
    - E.g.,  $\alpha_i = 2 \rightarrow$  count point twice

## Learning a Decision Stump on Weighted Data

#### Increase weight $\alpha$ of harder/misclassified points Credit Income Weight a 0.5 \$130K Safe Income? \$80K Risky 1.5 С 1.2 \$110K Risky Α \$110K Safe 8.0 \$90K Safe 0.6 Α > \$100K ≤ \$100K В \$120K Safe 0.7 C \$30K Risky 3 6.5 С \$60K Risky В \$95K Safe 8.0 Α \$60K Safe 0.7 Α \$98K Safe 0.9



### Boosting = Greedy Learning Ensembles from Data



# AdaBoost Algorithm



# AdaBoost: learning ensemble [Freund & Schapire 1999]

- Start with same weight for all points:  $\alpha_i = 1/N$
- For t = 1,...,T
  - Learn  $f_t(x)$  with data weights  $\alpha_i$
  - $\circ$  Compute coefficient  $\hat{w}_{t}$
  - $\circ$  Recompute weights  $\alpha_i$
- Final model predicts by:

$$\hat{y} = sign\left(\sum_{t=1}^{T} \hat{\mathbf{w}}_t f_t(\mathbf{x})\right)$$

# AdaBoost: Computing coefficient $\hat{w}_t$ of classifier $f_t(x)$

$$\frac{\text{Yes}}{\text{No}} \text{ in large}$$
No \text{ in small}

- $f_t(x)$  is good  $\rightarrow f_t$  has low training error
- Measuring error in weighted data?
  - Just weighted # of misclassified points



# AdaBoost: Formula for computing coefficient $\hat{\mathbf{w}}_t$ of classifier $f_t(x)$

$$\hat{\mathbf{w}}_t = \frac{1}{2} \ln \left( \frac{1 - weighted\_error(f_t)}{weighted\_error(f_t)} \right)$$





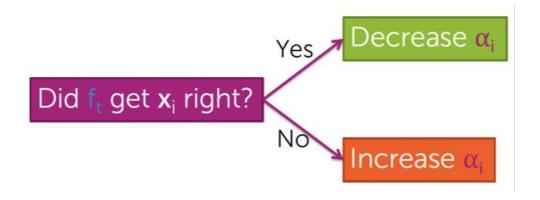
# AdaBoost: Learning Ensemble

- Start with same weight for all points:  $\alpha_i = 1/N$
- For t = 1,...,T
  - Learn  $f_t(x)$  with data weights  $\alpha$ i
  - $\circ$  Compute coefficient  $\hat{w}_{t}$
  - $\circ$  Recompute weights  $lpha_i$
- Final model predicts by:

$$\hat{\mathbf{w}}_t = \frac{1}{2} \ln \left( \frac{1 - weighted\_error(f_t)}{weighted\_error(f_t)} \right)$$

$$\hat{y} = sign\left(\sum_{t=1}^{T} \hat{\mathbf{w}}_t f_t(\mathbf{x})\right)$$

# AdaBoost: Updating weights $\alpha_i$ based on where classifier $f_t(x)$ makes mistakes





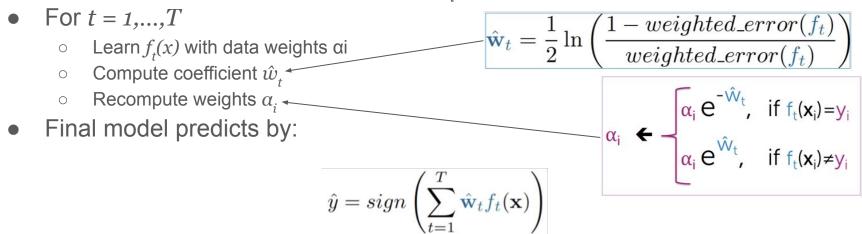
# AdaBoost: Formula for Updating Weights $\alpha_i$

$$\alpha_i \leftarrow \begin{cases} \alpha_i e^{-\hat{W}_t}, & \text{if } f_t(x_i) = y_i \\ \alpha_i e^{\hat{W}_t}, & \text{if } f_t(x_i) \neq y_i \end{cases}$$

	$f_t(x_i)=y_i$ ?	$\hat{W}_t$	Multiply $\alpha_i$ by	Implication
Did $f_t$ get $x_i$ right?				
No.				

## AdaBoost: Learning Ensemble

• Start with same weight for all points:  $\alpha_i = 1/N$ 



# AdaBoost: Normalizing Weights $\alpha_i$

If  $x_i$  often mistake, weight  $\alpha_i$  gets very large

If  $x_i$  often correct, weight  $\alpha_i$  gets very small

Can cause numerical instability after many iterations

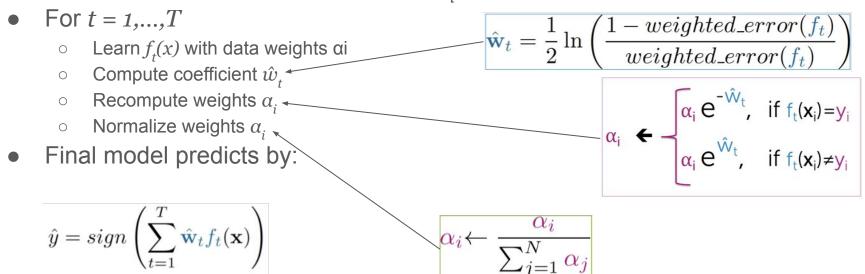
Normalize weights to add up to 1 after every iteration

$$\alpha_i \leftarrow \frac{\alpha_i}{\sum_{j=1}^N \alpha_j}$$



# AdaBoost: Learning Ensemble

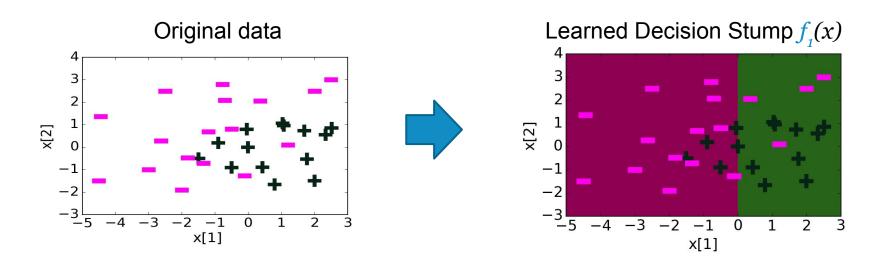
• Start with same weight for all points:  $\alpha_i = 1/N$ 



# AdaBoost Example: A Visualization

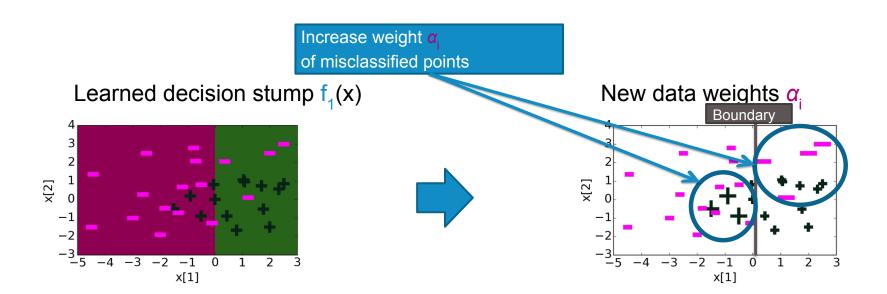


### *t*=1: Just Learn a Classifier on Original Data



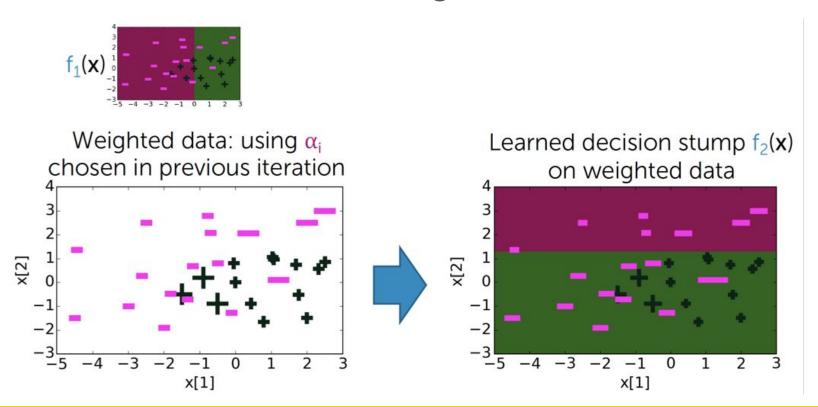


# Updating Weights $\alpha_i$



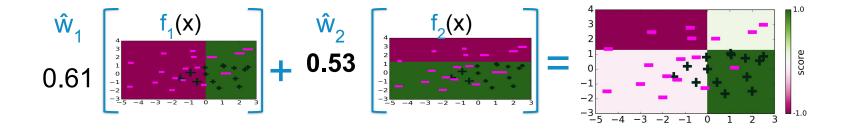


### *t*=2: Learn Classifier on Weighted Data

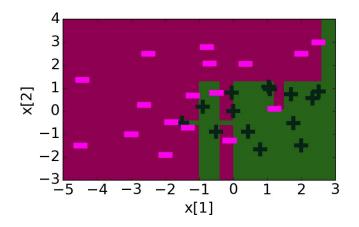




# Ensemble Becomes Weighted Sum of Learned Classifiers



# Decision Boundary of Ensemble Classifier after 30 Iterations



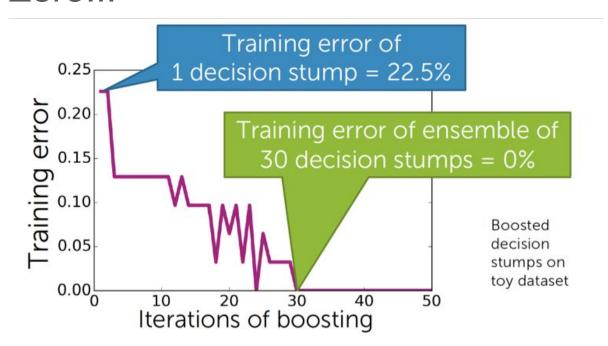
training\_error = 0



# **Boosting Convergence & Overfitting**



# After Some Iterations, Training Error of Boosting Goes to Zero!!!



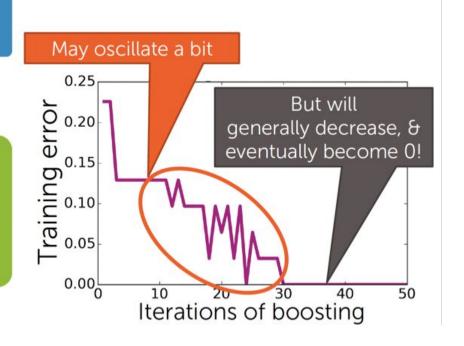


#### AdaBoost Theorem

Under some technical conditions...



Training error of boosted classifier  $\rightarrow$  0 as  $T\rightarrow\infty$ 



#### Condition of AdaBoost Theorem

Condition = At every t, Under some technical conditions... can find a weak learner with weighted\_error( $f_t$ ) < 0.5 Extreme example: No classifier can Not always separate a +1 on top of -1 possible Training error of boosted classifier  $\rightarrow 0$ Nonetheless, boosting often as T→∞ yields great training error



Training error of final classifier is bounded by:

$$\frac{1}{N} \sum_{i=1}^{N} \mathbb{I}[F(x_i) \neq y_i] \leq \frac{1}{N} \sum_{i=1}^{N} \exp(-y_i \mathbf{score}(x_i))$$

Where 
$$score(x) = \sum_{t} \hat{w}_t f_t(x)$$
;  $F(x) = sign(score(x))$ 

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Where  $\mathbf{score}(x) = \sum \hat{w}_t f_t(x)$ ;  $F(x) = sign(\mathbf{score}(x))$ 

Where  $score(x) = \sum_{t} \hat{w}_t f_t(x)$ ; F(x) = sign(score(x))

$$Z_{t} = \sum_{i=1}^{N} \alpha_{i,t} \exp(-\hat{w}_{t}y_{i}f_{t}(x_{i}))$$

$$Z_{t} = \sum_{i=1}^{N} \alpha_{i,t} \exp(-\hat{w}_{t}y_{i}f_{t}(x_{i}))$$

$$\alpha_i \leftarrow \frac{\alpha_i}{\sum_{j=1}^N \alpha_j}$$

If we minimize  $\prod_{t=1}^{T} Z_t$ , we minimize our training error

We can tighten this bound greedily by choosing  $\hat{w}_t$ ,  $f_t$  on each iteration to minimize:

$$Z_t = \sum_{i=1}^{N} \alpha_{i,t} \exp(-\hat{w}_t y_i f_t(x_i))$$

For boolean target function, this is accomplished by [Freund & Schapire '97]:

$$\hat{w}_t = \frac{1}{2} \ln \left( \frac{1 - \epsilon_t}{\epsilon_t} \right)$$

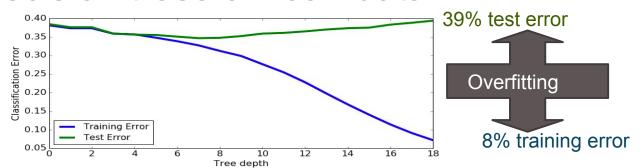
If each classifier is (at least slightly) better than random

$$weighted\_error(f_t) = \epsilon_t < 0.5$$

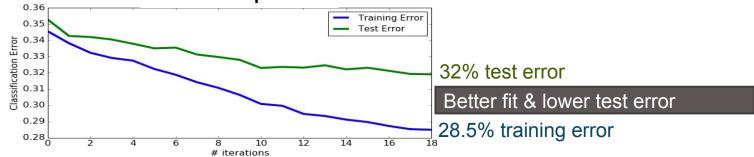
AdaBoost will achieve zero training error (exponentially fast):

$$\frac{1}{N} \sum_{i=1}^{N} \mathbb{I}[F(x_i) \neq y_i] \leq \prod_{t=1}^{T} Z_t \leq \exp\left(-2\sum_{t=1}^{T} (1/2 - \epsilon_t)^2\right)$$

#### Decision trees on loan data

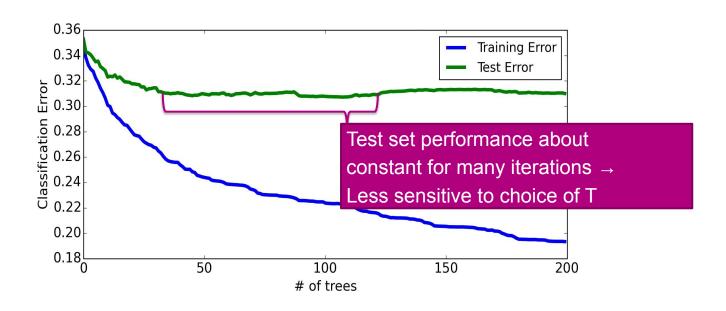


#### Boosted decision stumps on loan data



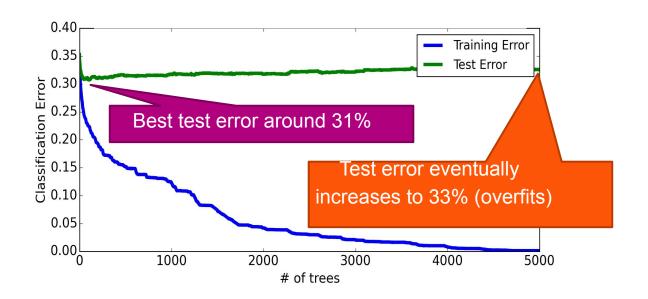


# Boosting Tends to Be Robust to Overfitting





# But boosting will eventually overfit, so must choose max number of components T





## Summary of Boosting

There are hundreds of variants of boosting, most important:

Gradient boosting

- Like AdaBoost, but useful beyond basic classification
- Great implementations available (e.g., XGBoost)

Many other approaches to learn ensembles, most important:

Random forests

- Bagging: Pick random subsets of the data
  - Learn a tree in each subset
  - Average predictions
- Simpler than boosting & easier to parallelize
- Typically higher error than boosting for same # of trees (# iterations T)



# Impact of Boosting (Spoiler Alert... HUGE IMPACT)

#### Amongst most useful ML methods ever created

Extremely useful in computer vision

• Standard approach for face detection, for example

Used by **most winners** of ML competitions (Kaggle, KDD Cup,...)

 Malware classification, credit fraud detection, ads click through rate estimation, sales forecasting, ranking webpages for search, Higgs boson detection,...

Most deployed ML systems use model ensembles

 Coefficients chosen manually, with boosting, with bagging, or others



#### What You Can Do Now...

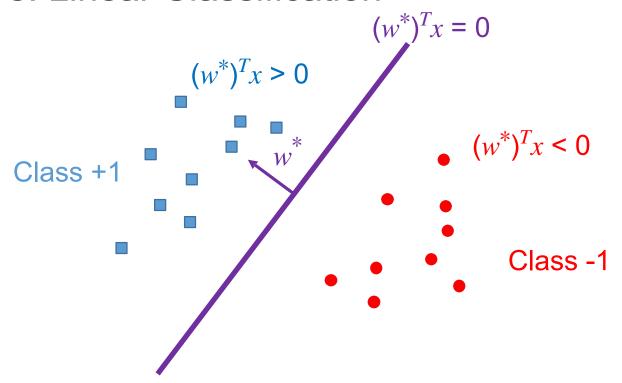
- Identify notion ensemble classifiers
- Formalize ensembles as weighted combination of simpler classifiers
- Outline the boosting framework sequentially learn classifiers on weighted data
- Describe the AdaBoost algorithm
  - Learn each classifier on weighted data
  - Compute coefficient of classifier
  - Recompute data weights
  - Normalize weights
- Implement AdaBoost to create an ensemble of decision stumps



# Support Vector Machine



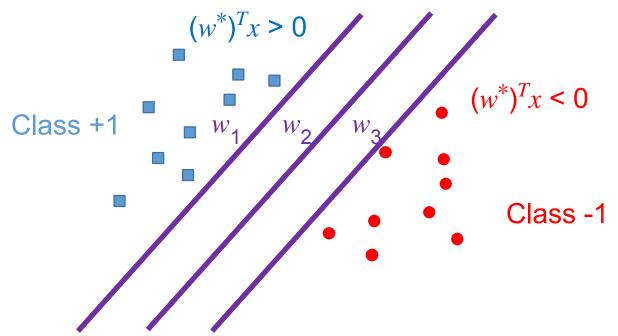
#### Motive: Linear Classification



Assume perfect separation between the two classes

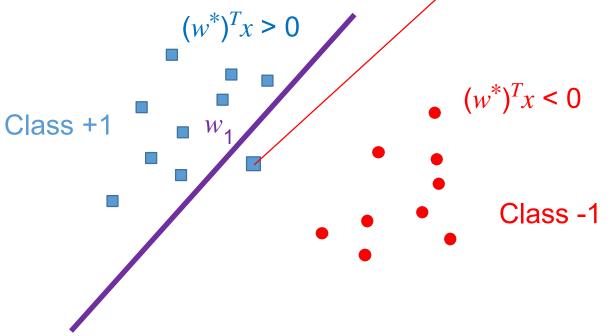


### Motive: Multiple Optimal Solutions?

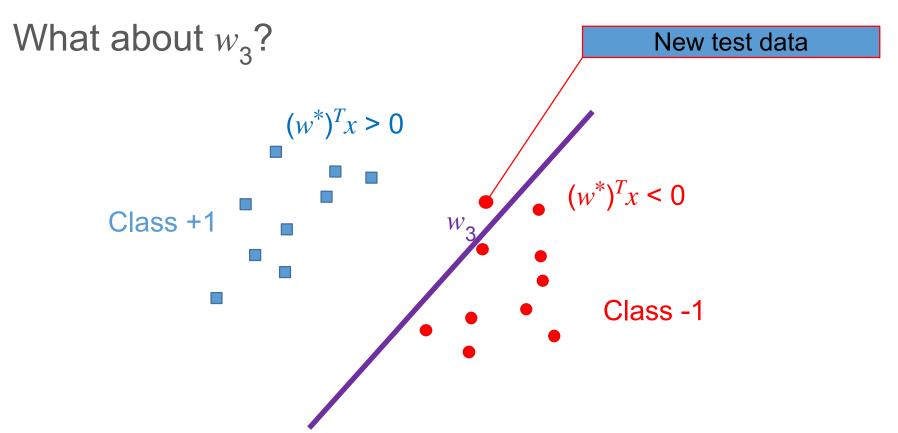




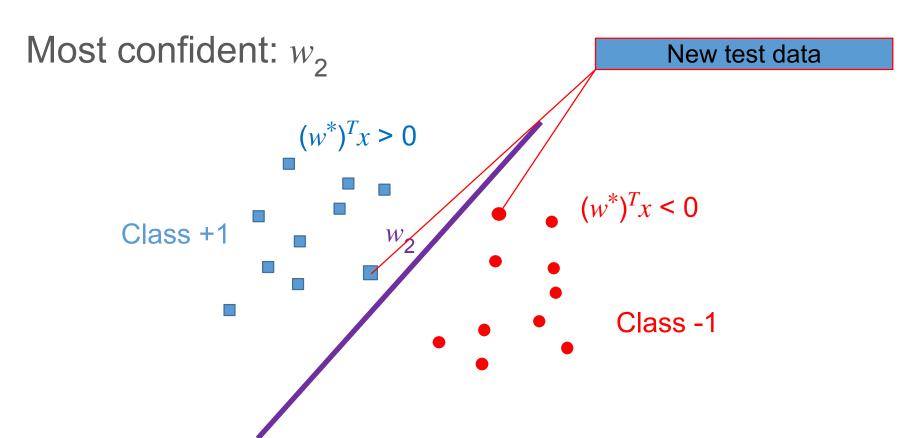
New test data



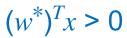


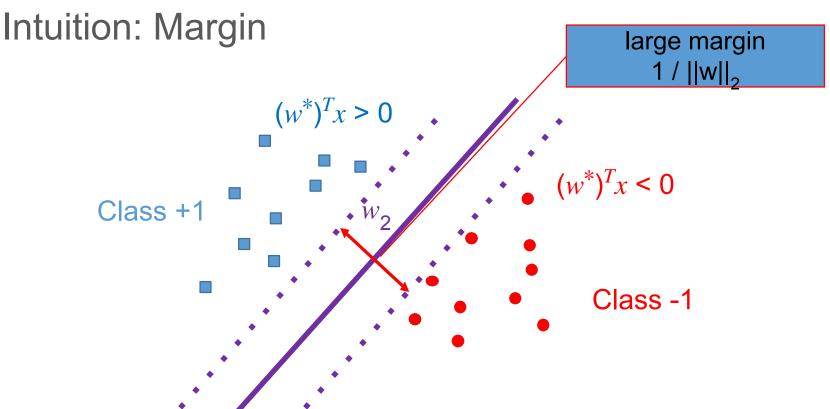




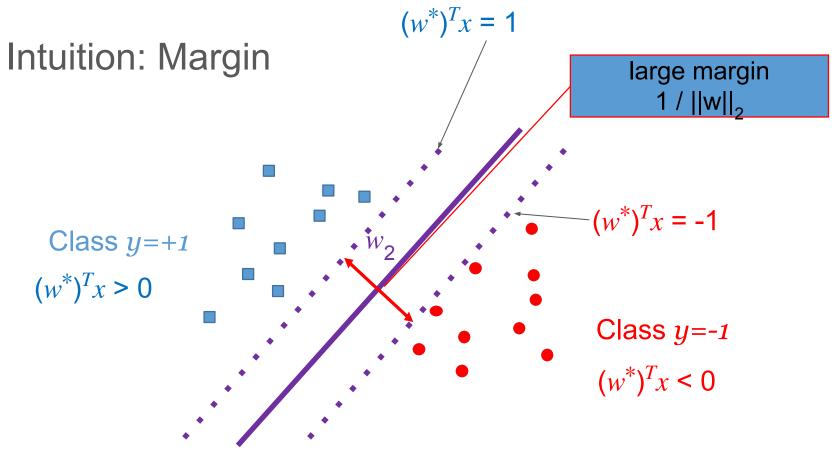










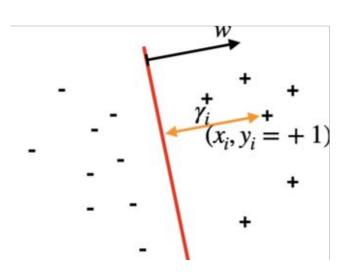




## **SVM: Geometric Margin**

- Given a set of training examples  $\{(x_i, y_i)\}_{i=1}^n$
- A linear classifier will be  $(w^*)^T x = 0$
- We define functional margin of w with respect to a training example  $(x_i, y_i)$  as the distance from the point  $(x_i, y_i)$  to the decision boundary, which is

$$\gamma_i = y_i \frac{(w^T x_i + b)}{\|w\|_2}$$



# Maximum Margin Classifier

We propose the following optimization problem, maximize the margin.

This is hard to do:

- maximize the numerator
- minimize the denominator

How about we just try to do this if we assume  $\gamma$  is a lower bound on the margin?

$$\gamma_i = y_i \frac{(w^T x_i + b)}{\|w\|_2}$$

$$\frac{\gamma_i(w^T x_i + b)}{\|w\|_2} \ge \gamma \quad \text{for all } i \in \{1, \dots, n\}$$

# Maximum Margin Classifier

Still hard to optimize, so we reparameterization if we condition the numerator is >=1:

$$\frac{y_{i}(w^{T}x_{i}+b)}{\|w\|_{2}} \ge \gamma \quad \text{for all } i \in \{1,...,n\} \longrightarrow \frac{\frac{y_{i}(w^{T}x_{i}+b)}{\|w\|_{2}}}{\|w\|_{2}} \ge \gamma \quad \text{for all } i \in \{1,...,n\}$$

Conditioning on  $y_i(w^Tx_i + b) \ge 1$  for all  $i \in \{1,...,n\}$ 

So we can see we want to maximize  $\frac{1}{\|w\|_2}$ , which is minimize  $\|w\|_2^2$ 

This is a quadratic problem with linear constraints, easy to solve

## Don't Forget It's Still a Classifier

We want to have a loss function that conditioning on the  $\ell(\hat{y}, y)$ 

So the overall SVM algorithm is try to optimize:

$$\lambda \|w\|_2^2 + \sum_{i=1}^n \mathcal{E}(\hat{y}, y)$$