2017 SDSC Summer Institute
Machine Learning Overview

SDSC SAN DIEGO SUPERCOMPUTER CENTER

UC San Diego

Classification

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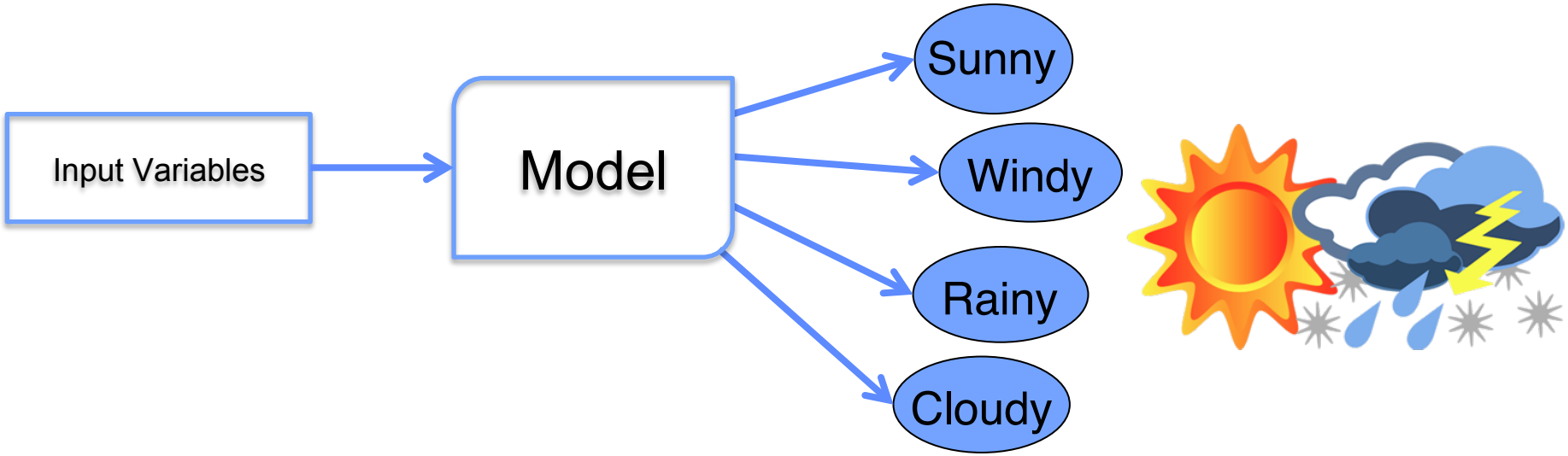
Overview

- **What is classification?**
- **Terminology & concepts**
  - Training and test sets
  - Generalization & overfitting
- **Classification Algorithms**
  - Decision Trees
  - Random Forest
  - Many others:
    - Naive Bayes, Logistic Regression, Neural Network, Support Vector Machines, etc.
- **Hands-on**
  - Build classification models for weather data

What is Classification?

- **Given input variables, predict target variable.**
  - Target variable is *categorical*.
  - Model needs to learn relationship between input data and target.
  - Other names for 'target'
    - label, class, class variable, output



Classification

Target variable

Input variables

RainTomorrow	Cloud9am	Pressure9am	Humidity9am	Temp9am
Yes	7	1019.7	68	14.4
Yes	5	1012.4	80	17.5
Yes	8	1009.5	82	15.4
Yes	2	1005.5	62	13.5
No	7	1018.3	68	11.1
No	7	1023.8	70	10.9

Classification Task: Can we predict the target variable from the input variables?

Note that classification is **supervised** learning.

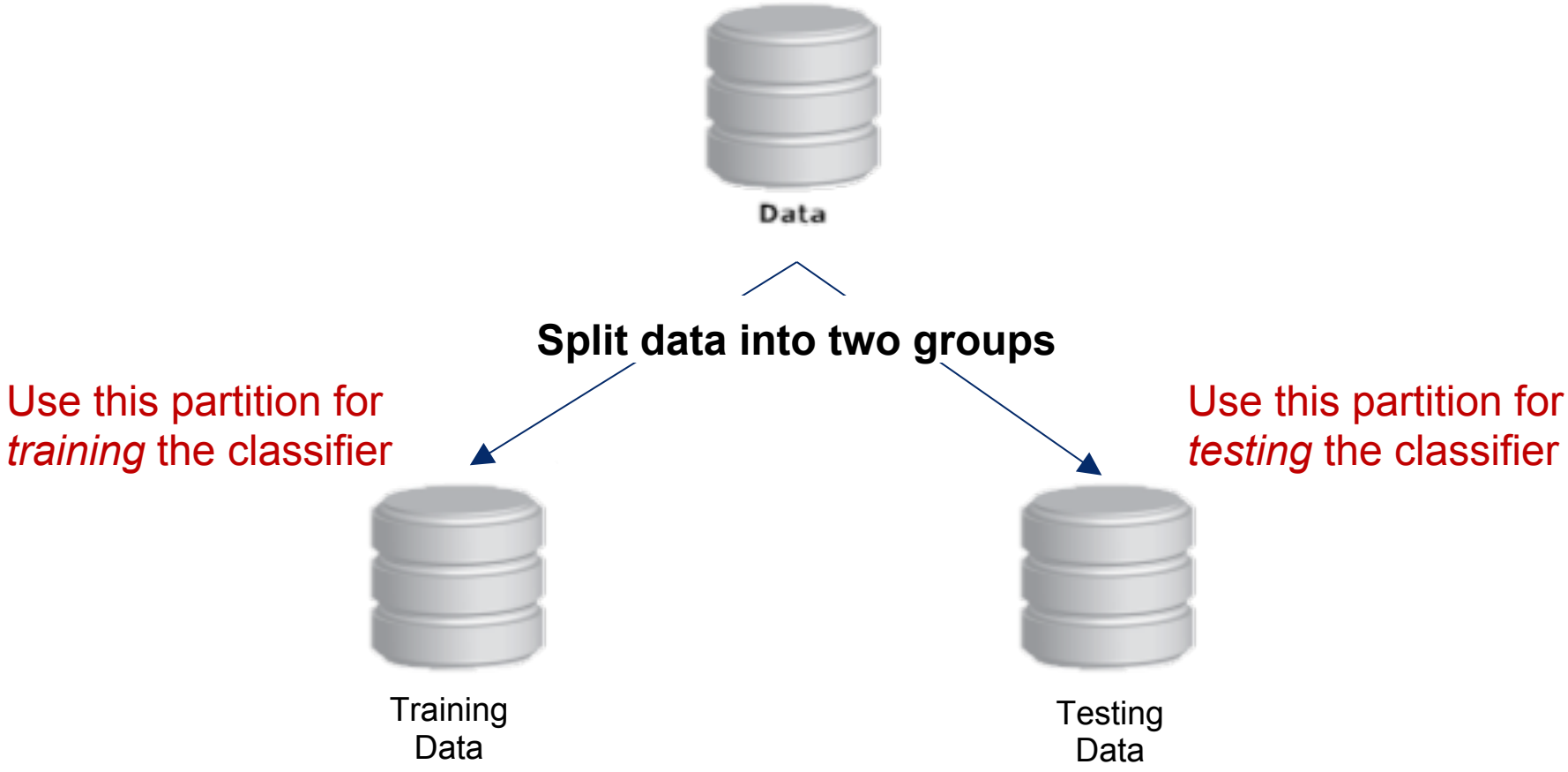
Target Variable in Classification

- **In classification, the target variable is always of categorical type.**
  - Binary Classification:
    - One of two classes for each sample
  - Multinomial or Multiclass Classification:
    - One of many classes for each sample
    - “many” = more than 2

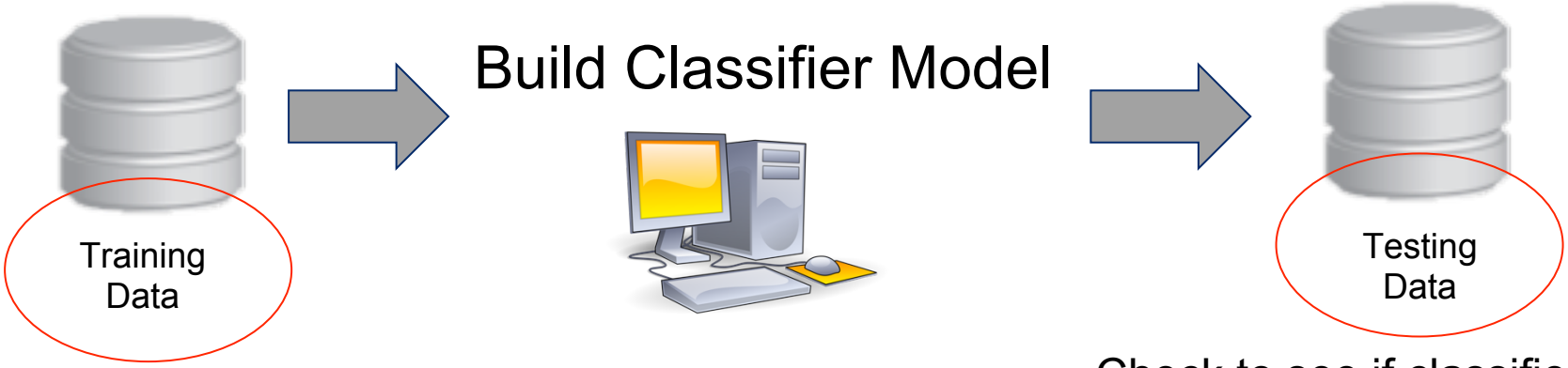
Building Classifier

- **In general, classifier is a mathematical model**
  - This model might not necessarily be a closed-form algebraic equation.
- **Classification model has a set of *parameters* that need to be *learned* or *estimated* from data.**
  - This is also referred to as “fitting the model”.
- **Usually, the more data we have, the better we are able to estimate the parameters.**

Generalization



Generalization

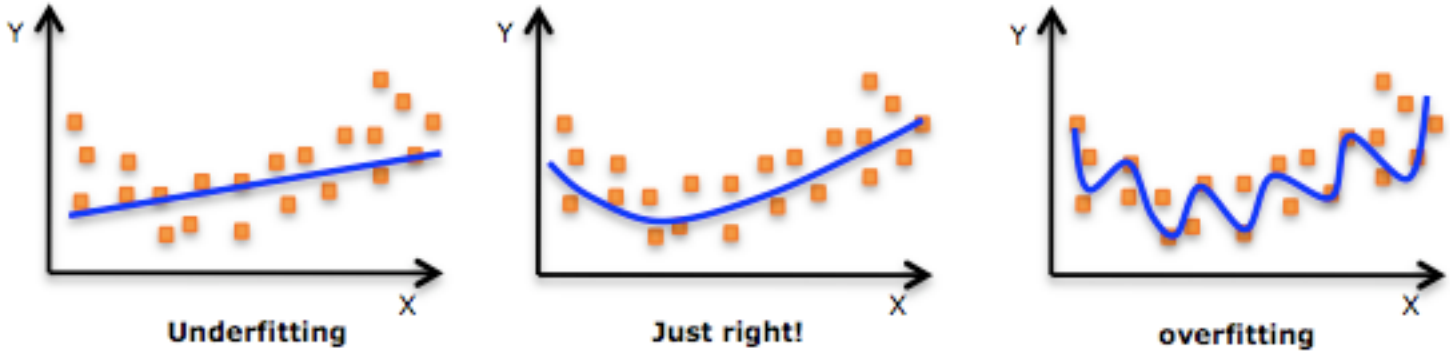


Check to see if classifier built is correctly classifying labels in *new* data

- **Build model on *training* dataset**
- **Test model on *test* dataset**

Overfitting

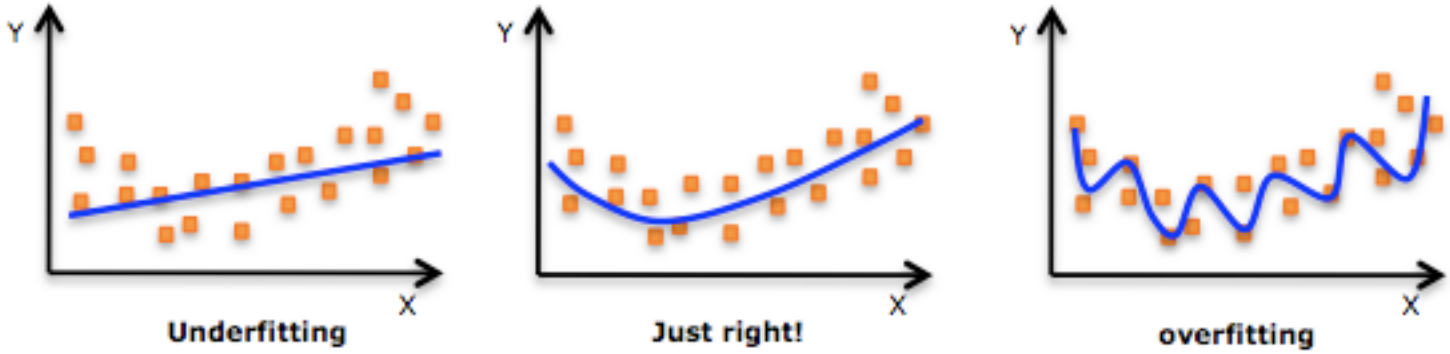
- *Overfitting* **occurs when model is fitting to noise in training data.**
- *Underfitting* **occurs when model has not learned structure of data.**



Source: http://stats.stackexchange.com/questions/192007/what-measures-you-look-at-the-determine-over-fitting-in-linear-regression

Overfitting & Generalization

- *Overfitting* **results in low training error & high generalization error.**
- *Underfitting* **results in high training error & high generalization error.**



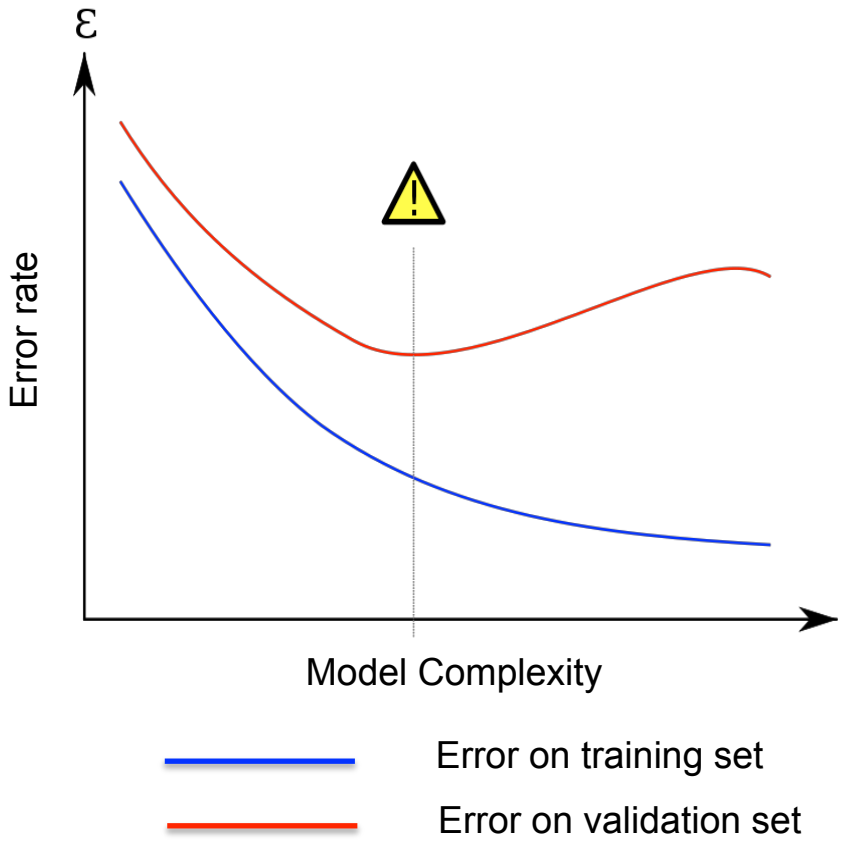
Source: http://stats.stackexchange.com/questions/192007/what-measures-you-look-at-the-determine-over-fitting-in-linear-regression

Overfitting & Generalization

- **To address overfitting and estimate generalization performance.**
- **Idea:**
  - Divide training set into multiple datasets
    - Training set: Used to fit model parameters to data
    - Validation set: Used to validate model performance
  - Monitor performance on training and validation sets to determine when to stop training.

Validation with Holdout Set

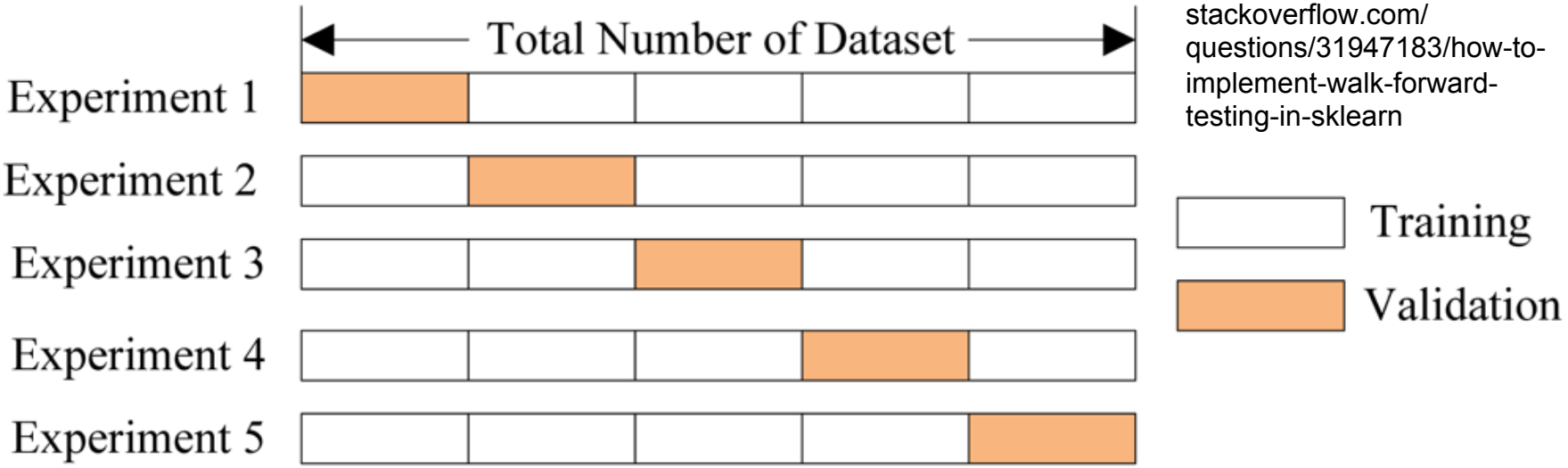
- Overfitting is occurring if training error decreases while validation error increases.
- Model with best generalization performance is one with lowest validation error.



Source: https://en.wikipedia.org/wiki/Overfitting

Cross-Validation

- **K-fold cross-validation**
  - Partition data into k disjoint datasets
  - For each iteration, use 1 partition for validation and the rest for training.
  - Repeat process k times. Each partition is used for validation exactly once.
  - Overall error estimate (generalization performance) is average of error rates for k iterations.

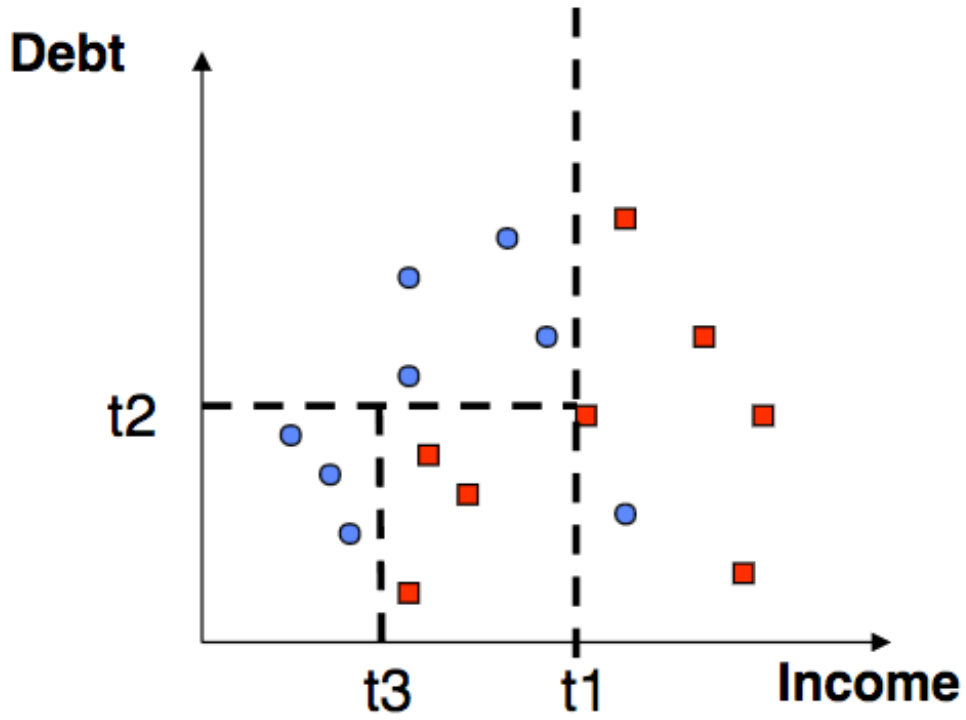


Source: http://stackoverflow.com/questions/31947183/how-to-implement-walk-forward-testing-in-sklearn

Decision Tree Overview

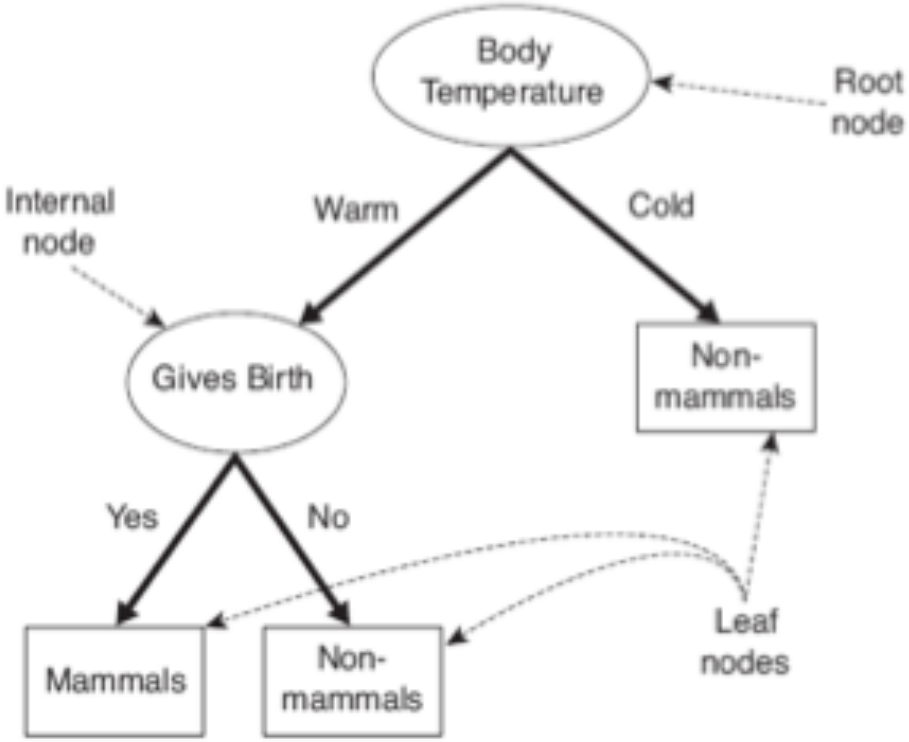
Can we split the data into cohesive groups?

- Split data into “pure” regions
- Classification decision based on these regions



Decision Tree Structure

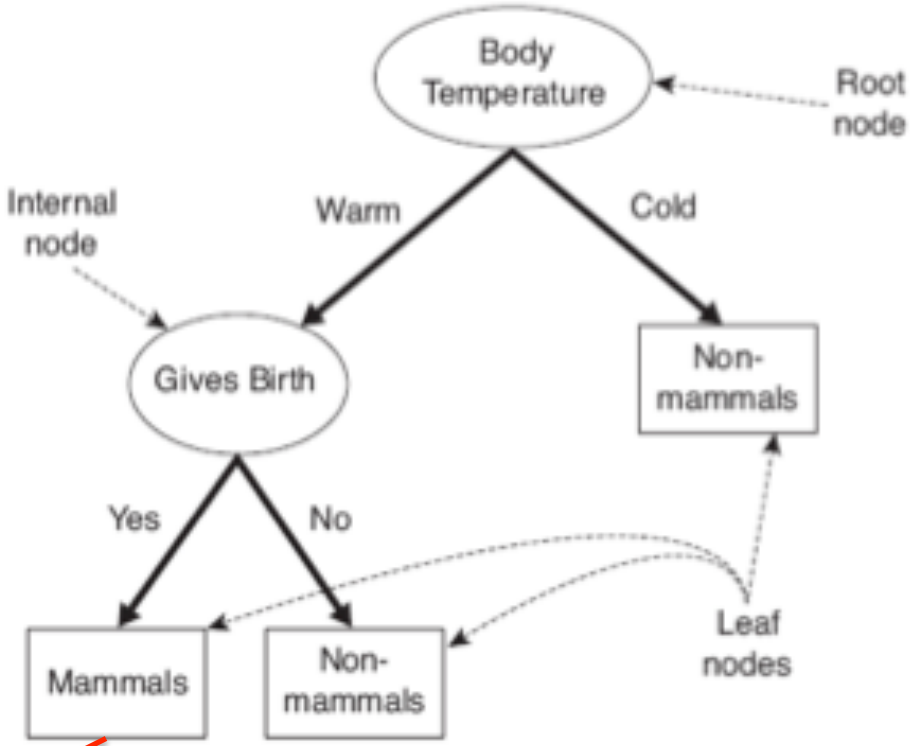
- Hierarchical structure with nodes and directed edges
- Root and internal nodes have test conditions.
- Leaf nodes have class labels.
- Paths from root to leaf represent classification rules.



Source: http://www-users.cs.umn.edu/~kumar/dmbook/dmslides/chap4_basic_classification.pdf

Classification Using Decision Tree

- Traverse tree from root to leaf.
- At each node, answer to test condition determines child node to move to.
- Category at leaf node determines label for sample.



Body Temp	Gives Birth	Target Label
Warm	Yes	Mammal

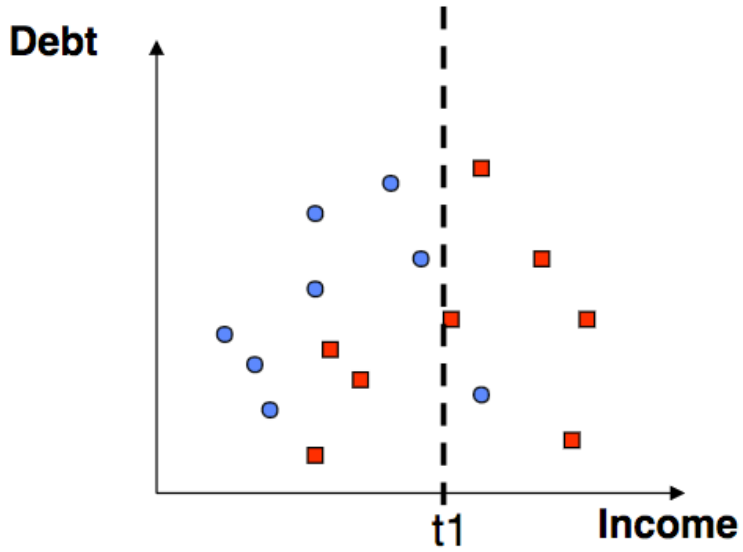
Source: http://www-users.cs.umn.edu/~kumar/dmbook/dmslides/chap4_basic_classification.pdf

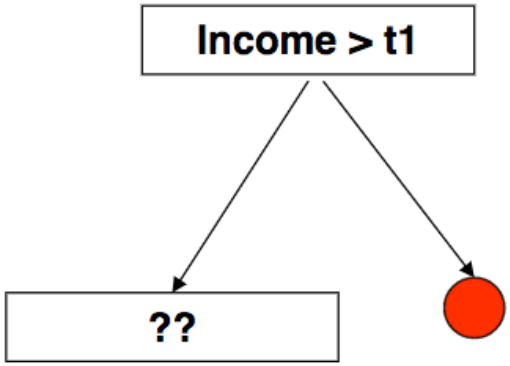
Constructing Decision Tree

- **Overview of tree induction:**
  - Start with all records at a node.
  - Partition records based on input variables.
    - Goal is to create subsets of records that are *purest* (i.e., most homogeneous) with respect to class distributions.
    - All possible splits on all input variables are considered and best split is determined.
  - Repeatedly partition data into successively purer subsets until stopping criteria are satisfied.

Decision Tree Example

- Split 1

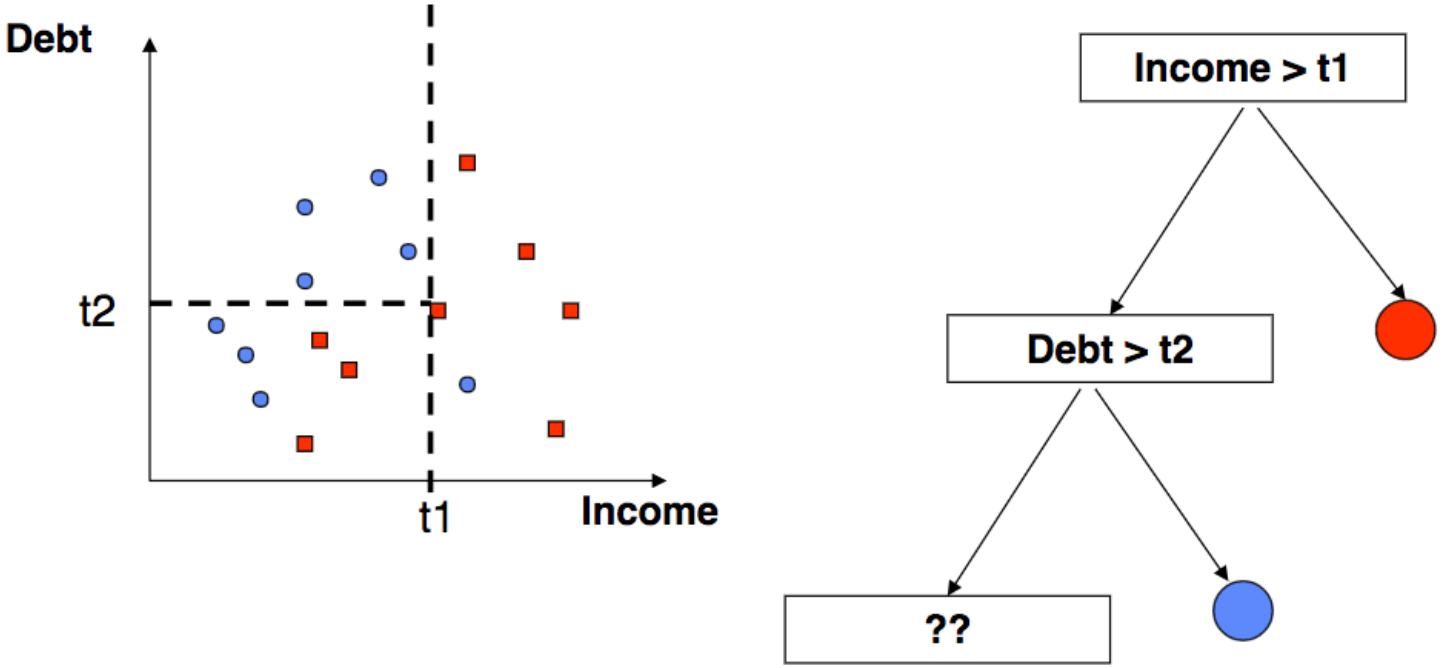




Source: https://www.ics.uci.edu/~rickl/courses/cs-171/cs171-lecture-slides/cs-171-19-LearnClassifiers.pdf

Decision Tree Example

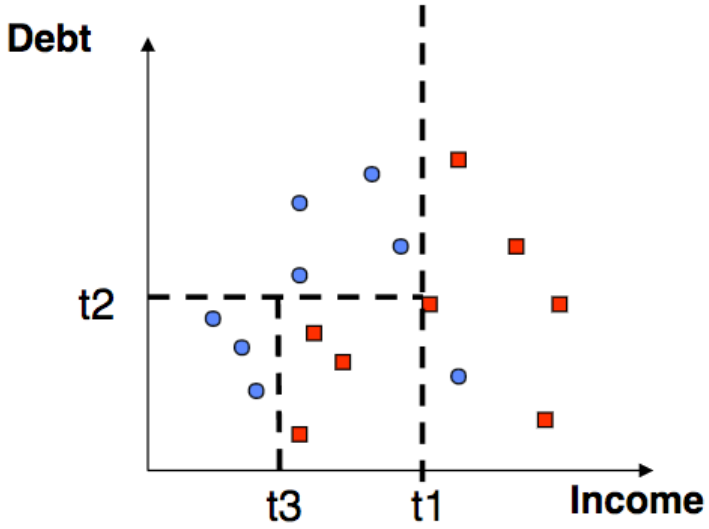
- Split 2

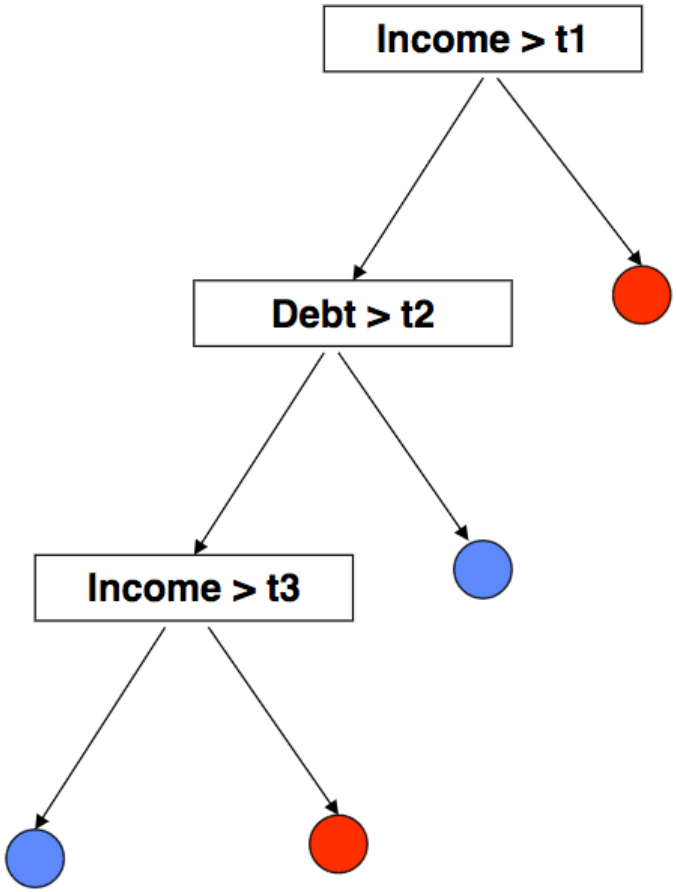


Source: https://www.ics.uci.edu/~rickl/courses/cs-171/cs171-lecture-slides/cs-171-19-LearnClassifiers.pdf

Decision Tree Example

- **Split 3**





More splits increases "purity" at the leaf nodes

Source: https://www.ics.uci.edu/~rickl/courses/cs-171/cs171-lecture-slides/cs-171-19-LearnClassifiers.pdf

Decision Tree Classification

- **Pros**
  - Resulting tree is often simple to understand and interpret.
  - Features can be any type (numerical or categorical), and can include missing values.
  - Tree induction algorithms are relatively computationally inexpensive.
- **Cons**
  - Induction algorithms use greedy approach where locally optimal decisions are made. No guarantee of globally optimal model.
  - Decision boundaries are rectilinear, limiting expressiveness for modeling complex relationships.

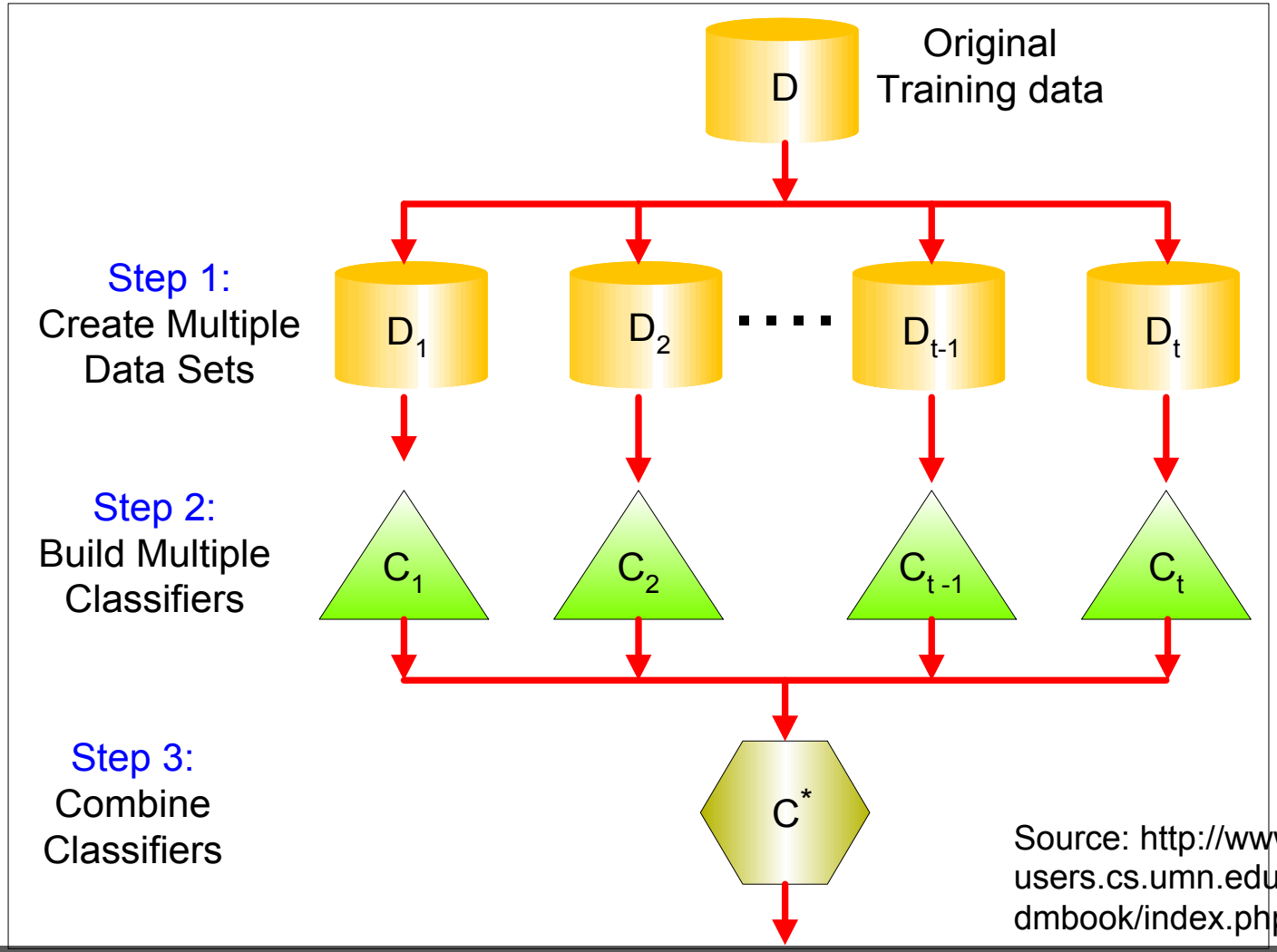
Random Forest

- **“forest”**
  - Ensemble method
    - Model is composed of set of decision trees => forest!
- **“random”**
  - For each tree, only subset of variables used to determine best split.
  - Subset of attributes is determined randomly.
- **Idea:**
  - To improve generalization of model

Ensemble Methods

- **Idea:**
  - Improve model performance by combining predictions of several models.
- **"ensemble":**
  - a group producing a single effect (from Merriam-Webster)
- **Approach:**
  - Construct a set of classifiers from training data.
  - Prediction is made by combining outputs of the multiple classifiers
    - Classification: Combine votes of classifiers

Ensemble Methods – Illustration



Ensemble Methods

- **Rationale for ensemble methods**
  - Consider ensemble that performs majority voting.
  - Base classifiers may make mistakes, but ensemble will misclassify a pattern only if over half of base classifiers are incorrect.
  - Intuitively, combining decisions from multiple “experts” may be more reliable than relying on a single “expert”.

Bagging

- **Bagging stands for "bootstrap aggregation".**
- **Approach:**
  - Sample training data set with replacement to construct bootstrap samples.
  - Build separate classifier on each bootstrap sample.
  - Each classifier predicts class label for unknown record.
  - Bagged classifier takes majority vote.
- **Generalization can be improved since variance of individual base classifiers is reduced.**

Random Forests – Revisited

- **Ensemble of decision tree classifiers.**
  - Base decision tree built by using only subset of attributes to determine split at each node.
    - Subset of attributes is determined randomly.
  - Bagging is used to generate bootstrap samples for base decision trees.
  - Final classification is based on the majority vote.
- **Randomization reduces correlation among base trees.**
  - Generalization of ensemble can be improved.

Randomness in Random Forest

- **Randomness can be incorporated in several ways:**
  - Forest-RI
    - Random attribute selection: At each node, randomly select subset of input attributes to consider in splitting node.
  - Forest-RC
    - Random combinations of attributes: At each node, randomly select subset of input attributes to be linearly combined. These new attributes are considered in splitting node.
  - Randomly select best split:
    - At each node, randomly select one of F best splits.

Random Forest Classification

- In practice, often results in improved performance due to lower variance.
- Training takes longer.
- Ensembles more difficult to understand than single classifiers.

Classification – Key Points

- **Classification task**
  - Predict categorical variable from input variables
- **Overfitting & Generalization**
  - Avoid overfitting to have model generalize to new data
  - Techniques: validation with holdout set, cross-validation
- **Algorithms**
  - Decision Trees, Random Forest
  - Others: k-nearest-neighbor, naïve Bayes, neural networks, …

References

- A. Liaw et al. Package 'randomForest'. Retrieved from https://cran.r-project.org/web/packages/randomForest/randomForest.pdf
- P. Tan, M. Steinbach, & V. Kumar. *Introduction to Data Mining*. Pearson: 2005.
- T. Therneau, B. Atkinson, & B. Ripley. Package 'rpart'. Retrieved from https://cran.r-project.org/web/packages/rpart/index.html

Questions?