Supervised learning. Decision tree learning (DTs)

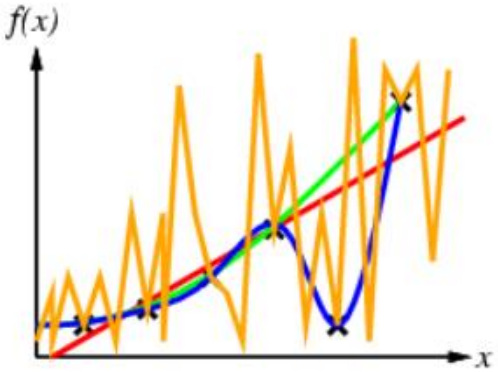
SUMMARY

1. Issues in ML

- what algorithms can approximate functions well (and when)?
- how does the number of training examples influence performance?
- how does complexity of hypothesis representation impact learning performance?
- how does noisy data influence performance?
- what are the theoretical limits of learnability?
- …

2. Supervised learning

- example: Inductive learning
- learn a function from examples
- Occam's razor
  - prefer the simplest hypothesis consistent with data
  - complex models tend not to generalize well



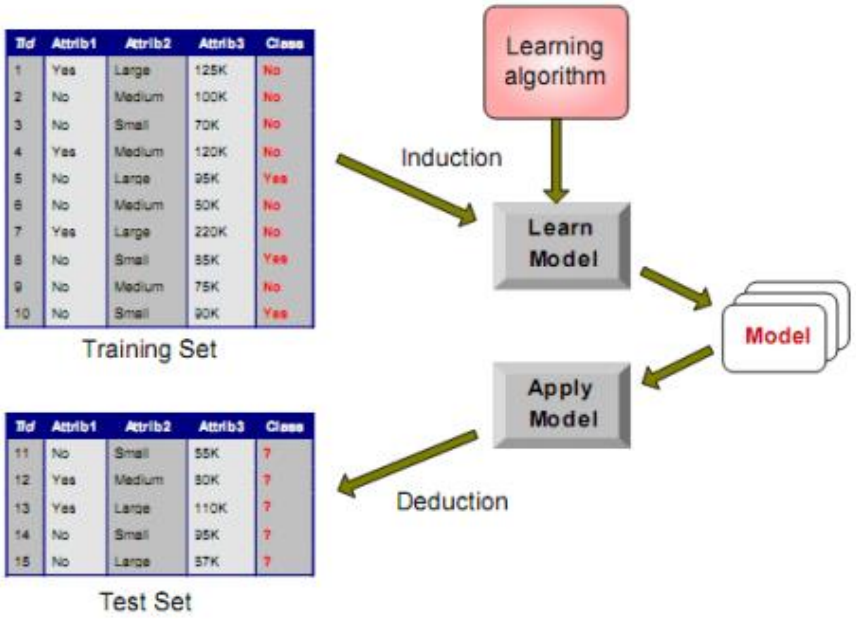
[2]

- **Classification** vs. **regression**
    1. learning a relationship between an input (vector *x*) and an output (*y*) from data
    2. **classification** estimates the discrete output *y* (known as the class)
        - **types**
            - One Class Classification (OCC)
                - Imbalanced data
                - Anomaly/outlier detection, open set recognition (OSR)
                - E.g., OSVM,…
            - Binary classification
            - Multi-class classification
        - predicting tumor cells as benign or malignant
        - categorizing news according to their domain (finance, sports, weather, etc)
        - classifying secondary structures of proteins
        - classifying credit card transactions
        - ….
    3. **regression** estimates the function **f** such that $y=\mathbf{f}(x)$ with some confidence measure
        - predicting the exchange rate
        - predicting the price of houses
        - predicting the age of a person
        - …..
- **Offline vs. online** learning
    1. **Offline (batch) learning**
        - generates the best predictor by learning on the entire data set at once
    2. **Online learning**
        - data becomes available in a sequential order and is used to update the best predictor for future data at each step
        - learning incrementally (one instance at time)
        - useful where is computationally unfeasible to train over the entire data set (e.g. stock price prediction)
        - time dependent
- **Eager** vs. **lazy** learning
    1. **Eager learning**
        - an example of offline learning
        - the system tries to construct a general, input independent target function during the training of the system
            - a global model (hypothesis) is built during the training step
            - slow training, fast evaluation
        - builds a global estimate of the target function
        - deal much better with noise
        - generally unable to provide good local approximations of the target function
        - e.g. ANNs, SVMs, DTs, NBC, etc
    2. **Lazy learning**
        - little or no offline processing of the training data
        - motivation
            - online learning
            - data set is continuously updated with new entries

- generalization beyond the training set is delayed until a query is made to the system
- simply stores the training examples
  - not really a training phase
  - fast "training", slow evaluation
- e.g. instance-based learning methods (kNN, LWR, CBR)
  - e.g., kNN used in online recommendation systems (movies, music, items to sale, a.s.o)
- provide a local approximation for the target function, for each new query instance

3. Eager inductive learners

- Most of the inductive learning models are eager ones.
- Building an eager inductive learner



[2]

- train-validation-test sets
- e.g., 60-20-20 split

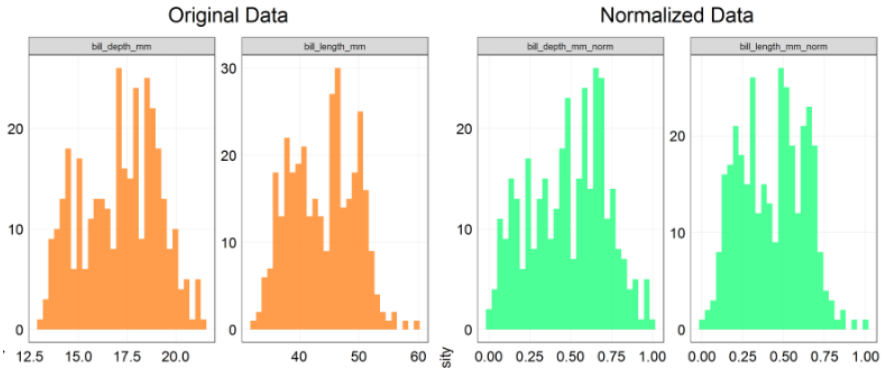
Data pre-processing and analysis

- data cleaning (cleansing)
- **normalization/standardization** (for numerical data), if needed
  - if X is a feature characterizing the data, $X = (X_1, X_2, \dots X_n)$
  - normalization and standardization will not change the distribution of the data
  - **(min-max) normalization**

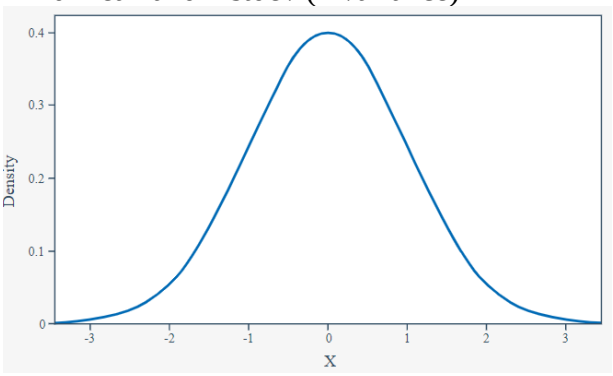
- changes the range of the data (i.e., the relative distances between individual data points)
  - does not alter the data distribution
- scale the data between 0 and 1

$$X_i' = \frac{X_i - min}{max - min}$$

  - where *min* and *max* represent the *minimum* and *maximum* values of *X*
  - useful in ML algorithms that do not assume any distribution of data (kNN, neural networks).



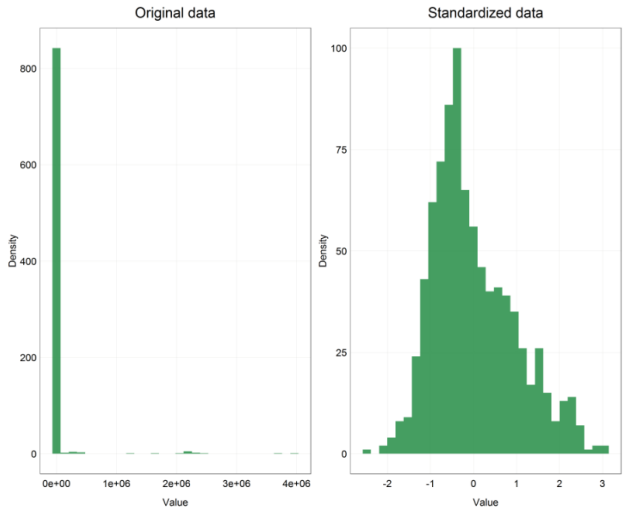
- **standard deviation-based normalization (*standardization*)**
  - standard normal distribution *N*(0,1)
    - 0 mean and 1 stdev (1 variance)



  - after standardization the data will have zero mean and unit variance

$$X_i' = \frac{X_i - \mu}{\sigma}$$

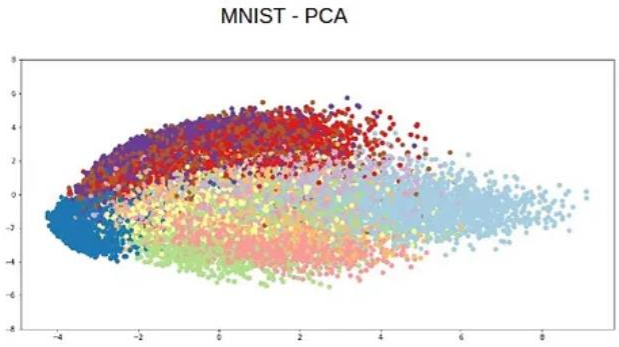
    - μ represents the mean and σ represent the standard deviation of X
  - preserves the general data distribution
    - shifts and scales a distribution
    - it does not change the shape of the distribution

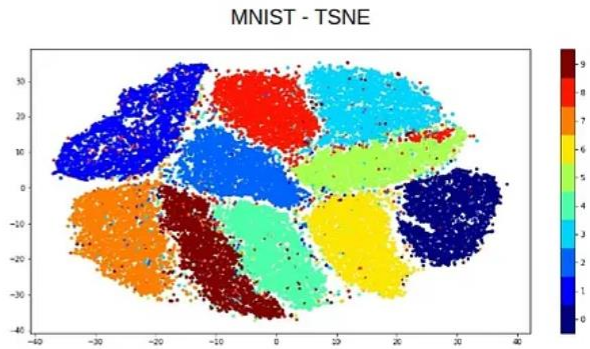


- the transformed data are now centered on 0

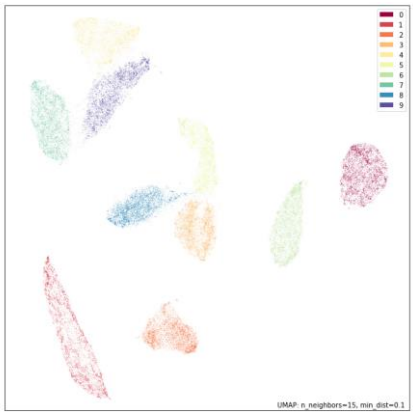
- **feature selection**
  - **select relevant features**
    - correlation
    - independence tests
      - Pearson's χ^2 test
    - unsupervised learning
      - univariate filter methods
        - information theory, spectral analysis (manifold learning)
    - **univariate feature selection**
      - feature importance – statistical tests
      - select the most important features in a dataset
      - evaluate a feature's relationship with the target variable and select the ones that have the strongest correlation
      - *scikit-learn*
        - F-test for feature scoring
    - algorithms: Relief-based
      - *scikit-learn*
- **component reduction**
  - build new input variables in order to reduce their number
  - no loss of information about data distribution
  - data vizualisation tools
  - **Principal Component Analysis** (PCA)
    - map data into a space of lower dimensionality
    - linear mapping
    - preserving as much of the data's variance
  - **Curvilinear Component Analysis** (CCA)
    - non-linear extension of PCA
    - is a kind of self-organizing map
  - **t-Distributed Stochastic Neighbor Embedding** (t-SNE)
    - non-linear dimensionality reduction

- **Uniform Manifold Approximation and Projection for Dimension Reduction** (UMAP)





MNIST-UMAP



- **others**
  - outliers, isolated instances
  - **imbalanced data**
    - data augmentation
      - oversampling
        - SMOTE (Synthetic Minority Oversampling TEchnique)
        - Cluster-based oversampling (CBOS)
        - Others
      - generative oversampling
        - GANs, VAE-based
    - undersampling
      - algorithms/rules for deciding the examples to keep from the majority class
      - e.g., Condensed Nearest Neighbors

Build the model (training) – *induction*

- **training set**
  - used to train the model

- **validation set** (extracted from the training data) can be used for optimizing the model
  - used to validate the model
    - on data unseen during training
  - unbiased evaluation of a model fit on the training dataset while tuning the model's hyperparameters.
  - **cross-validation** may be used
  - "best" model

Evaluate/test the performance of the model

- **test set**
  - unbiased evaluation of a final model fit on the training data set
- apply the model – *deduction*
- for evaluating the performance of the model, a cross-validation (**CV**) testing methodology should be used
- **CV**
  - helps in detecting overfitting
  - a way to test robustness
  - a statistical analysis of the results obtained during the CV (e.g., **confidence intervals - CIs**)
    - **Central Limit Theorem** for Cross-validation
      - given a sufficiently large sample size, the sampling distribution of the mean for a variable will approximate a normal distribution
    - perform multiple independent (or close to independent) evaluations of a model performance to result in a population of estimates
      - the mean of these estimates will be an estimate (with certain error) of the true underlying estimate of the model skill on the problem
    - around 30–50 repetitions for computing **CI**s
  - multiple (training-validation-testing) splits are used
    - *k*-fold cross-validation
      - *k* buckets
        - *k*-1 used for training, the remaining for testing
        - repeat *k* times
          - *k* performance measures $P_1, P_2, \dots, P_k$
        - μ - the mean performance
          - $\mu = \frac{\sum_{i=1}^{k} P_i}{k}$
        - compute the **CI** of μ
          - $[\mu - \alpha, \mu + \alpha]$ (or $\mu \pm \alpha$)
          - α is the *confidence value*
          - e.g., for 95% CI

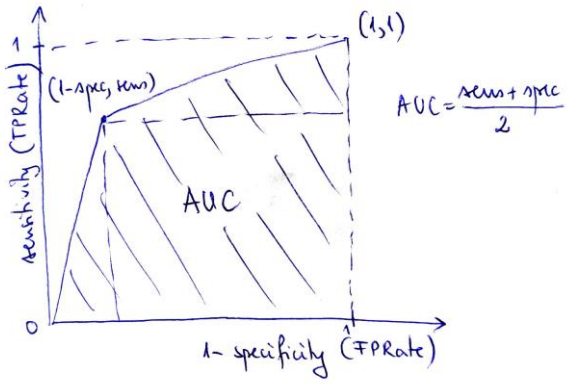
$$\alpha = 1.96 \cdot \frac{\sigma}{\sqrt{k}}$$

        - 10 is usually used for *k*
    - leave-one out cross-validation
        - *n*-1 instances for training, the remaining for testing
        - repeat *n* times
        - only one performance measure is provided
            - *accuracy*
        - computationally expensive
    - "2/3-1/3" split
        - randomly select 2/3 from the data for training, the remaining for testing
        - repeat *k* times
        - CI of the mean performance

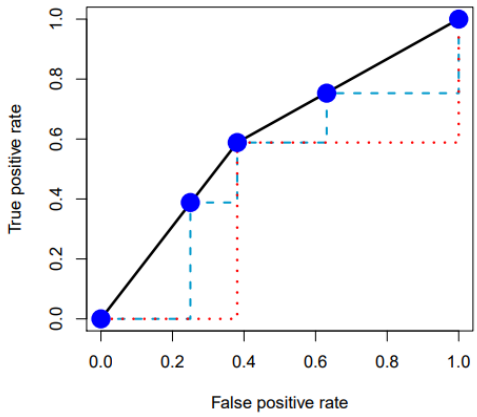
- performance measures used for assessing the performance of a ML model:
    - **for classification**:
        - accuracy, precision, recall (sensitivity), f-measure (f-score), specificity, AUC (Area under the ROC curve), AUPRC (Area under the precision/recall curve)
            - [0,1]
            - binary classification
                - confusion matrix (computed on a testing data set)
                    - TP - # of true positives
                    - TN - # of true negatives
                    - FP - # of false positives
                    - FN - # of false negatives

$acc = \frac{TP + TN}{TP + TN + FP + FN}$	$prec_+ = \frac{TP}{TP + FP}$ (Positive predictive value, PPV)	$sens = recall_+ = \frac{TP}{TP + FN}$ (TPRate, probability of detection - POD)
$f\text{-}score_+ = \frac{2}{\frac{1}{prec_+} + \frac{1}{recall_+}}$	$prec_- = \frac{TN}{TN + FN}$ (Negative predictive value, NPV)	$spec = recall_- = \frac{TN}{TN + FP}$ (TNRate)
$f\text{-}score_- = \frac{2}{\frac{1}{prec_-} + \frac{1}{recall_-}}$	$f\text{-}score = \frac{f\text{-}score_+ + f\text{-}score_-}{2}$	Weigthed f-score

- higher values are better
- accuracy (*acc*)
    - *n* is the dimensionality of the testing data
    - $acc = \frac{1 + 0 + \cdots + 1}{n}$
    - 95% CI of *acc* (the mean of a population parameter)
        - $\alpha = 1.96 \cdot \sqrt{\frac{acc \cdot (1 - acc)}{n}}$
- **AUC**
    - imbalanced data
    - only one point on the ROC (Receiver Operating Characteristic) curve

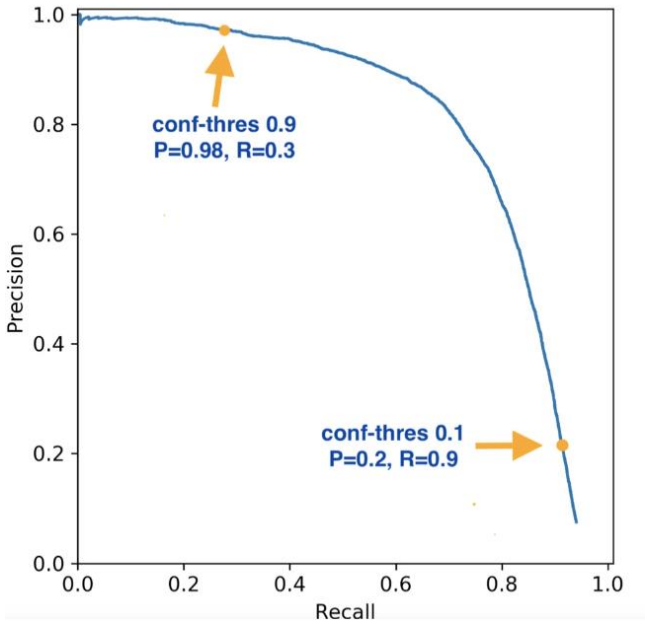


    - multiple points



    - performance of the classifier
        - AUC=0.5 random classifier
        - AUC $\in$(0.5,0.6] poor
        - AUC $\in$(0.6,0.7] fair
        - AUC $\in$(0.7,0.8] good
        - AUC $\in$(0.8,0.9] very good
        - AUC $\in$(0.9,1] excellent

- **AUPRC**
  - Area under the Precision-Recall curve



- **other**
  - e.g., (weather) forecasting
    - critical success index (CSI)
    - false alarm rate (FAR)
    - BIAS
    - HSS (Heidke Skill Score)
    - etc

- multi-class classification
  - generalization from the binary case
  - $M=(m_{i,j})_{i,j=1,n}$ where n is the number of classes
    - generalization from the binary case
    - $m_{i,j}$= number of instances having the actual class j, predicted as belonging to class i
    - the evaluation measures are computed for each class i (e.g., $prec_i$, etc)
      - an aggregated measure is provided

- **for regression**: MAE (Mean of Absolute Errors), RMSE (Root Mean Squared Error), NRMSE (Normalized Root Mean Squared Error), R^2 (R-squared - coefficient of determination)
  - MPE (Mean percentage error)
  - MAPE (Mean absolute percentage error)
    - forecasting
  - lower values are better
    - e.g., NRMSE below 5%

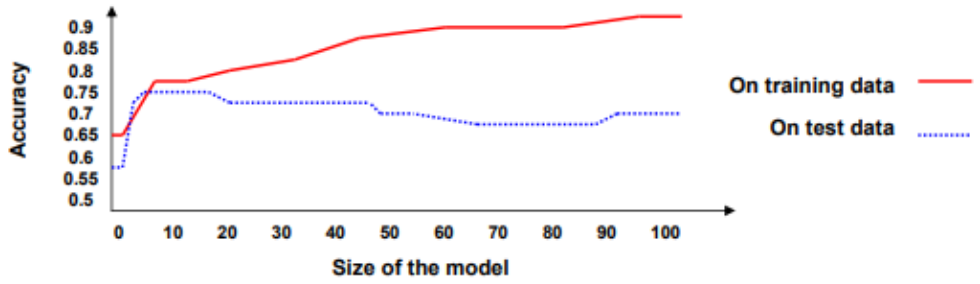
$MAE = \frac{\sum_{i=1}^{n} \lvert y_i - f(x_i) \rvert}{n}$ y_i - predicted value for x_i $f(x_i)$ - true value (observation – in forecasting) n - # test instances	$RMSE = \sqrt{\frac{\sum_{i=1}^{n} (y_i - f(x_i))^2}{n}}$
$MAPE = \frac{100\%}{n} \cdot \sum_{i=1}^{n} \lvert \frac{f(x_i) - x_i}{f(x_i)} \rvert$	$R^2 = 1 - \frac{SS_{RES}}{SS_{TOT}} = 1 - \frac{\sum_i (y_i - \hat{y}_i)^2}{\sum_i (y_i - \bar{y})^2}$ • y – observations • $\hat{y}$ - predictions

- comparing the performance of two classifiers/regressors
  - **confidence intervals**
  - **statistical tests**
    - is there a statistically significant difference between the performances of 2 models?
      - one/two-tailed Wilcoxon signed rank test for paired data, …

Generalization

1. overfitting

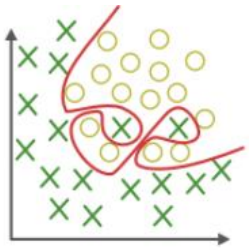
- overfitting is finding complex functions due to
  - small number of training instances
  - noise or irrelevant data
- a hypothesis overfits the training data if a hypothesis that fits the training examples less well performs better on the entire data distribution
- an overfit model performs well on the training set, but usually has poor generalization capabilities



[2]

- causes
  - the model is too complex
    - models the training data two well
    - does not generalize

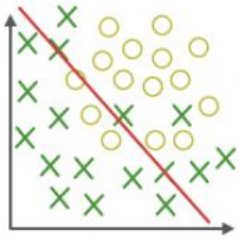
- the training data is relatively small and is an insufficient representation of the underlying distribution that it is sampled from
    - the model fails to learn a generalizable mapping.



- good performance on training data but poor performance on testing data
- techniques to reduce overfitting:
    - Increase training data.
    - Reduce model complexity.
    - Early stopping during the training phase.
        - stop training once the model performance stops improving on a hold-out validation data set
    - Use regularization techniques (L2, L1 - Ridge Regularization, Lasso Regularization)
        - reducing the generalization error without affecting the training error much
    - Use dropout for neural networks to tackle overfitting.

2. underfitting

- the model is too simple

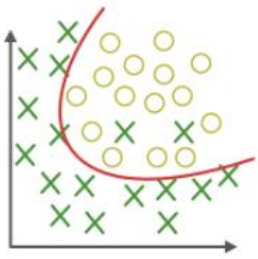


- a model that can neither model the training data, nor generalize to new data
- poor performance both on training data and on testing data

Overfitting and underfitting

- causes for poor performance of ML models

3. **appropriate fitting**

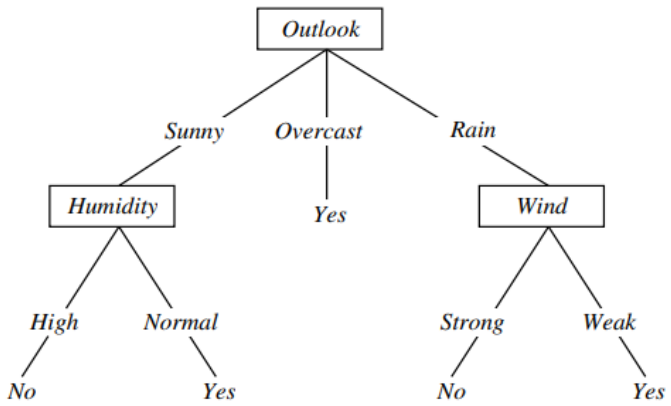


4. Decision tree (DT) learning

- **recent advances**
  - Deep DTs (**Decision Streams**)
    - deep directed acyclic graph of decision rules
  - Deep neural DTs
  - Deep neural decision forests
  - „**Awesome DT research papers**“ - https://github.com/benedekrozemberczki/awesome-decision-tree-papers

- used in Data Mining and Machine Learning, uses a decision tree as a predictive model
  - one of the practical methods for inductive inference
- it can be used both for classification and regression
- is an eager inductive learning model
- DT algorithms
  - ID3 – offline algorithm (Iterative Dichotomiser 3, Ross Quinlan in 1986)
  - ID4 is the online variant of ID3
  - C4.5 (C5.0) extensions of ID3
  - J48 is an open source Java implementation of C4.5 in Weka
  - CART (Classification And Regression Trees)
  - aso
- follows the principle of **Occam's razor** in attempting to create the smallest DT possible
- **Limitations**
  - the problem of learning an optimal DT is NP-complete ⇒ the greedy algorithms lead to a local optimum
    - *n* boolean attributes/features, binary classification ⇒ how many distinct trees?
  - overfitting (complex trees)
  - the DT model is **unstable (**small fluctuations in data can make a large difference)
    - bagging, boosting
- **Advantages**
  - simple to understand and interpret
    - people are able to understand DT models
      - interpretable/explainable ML (XML)
        - making ML models and their decisions interpretable
    - uses a white box model
  - require little data preparation (other techniques often require data normalization, missing values to be removed)
  - able to handle both numerical and categorical data

        - **categorical variables**
            - fixed number of possible values
            - information can be sorted in categories
            - types of categorical variables
                - *ordinal* (some intrinsic order between the values, e.g. **rating**: excellent, good, fair, poor)
                - *nominal* – without any intrinsic order (e.g. **sex**: male, female)
                - *binary* (true, false)
        - **continuous variables**
            - can take an infinite number of possible values **(**e.g. real numbers)
            - e.g. temperature, blood pressure
    - perform well with large data sets
- **Decision tree representation**
    - each internal node tests an attribute
    - each branch corresponds to an attribute value
    - each leaf node assigns a classification
    - in DT learning, a hypothesis is a *decision tree*
    - DT classify instances by sorting them down the tree from the root to some leaf node, which provides the classification of the instance

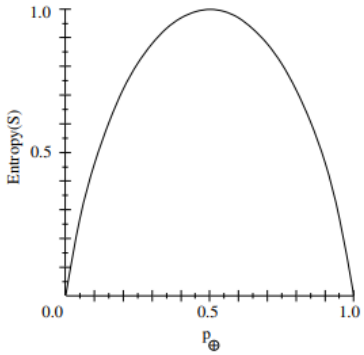


[1]

- DT – disjunctive expression
    - (*Outlook=Sunny* ∧ *Humidity=Normal*) ∨ (*Outlook=Overcast*) ∨ (*Outlook=Rain* ∧ *Wind=Week*)
- hypothesis in DT learning is a *decision tree* (model)

- **When to consider DTs**
    - instances describable by attribute-value pairs
    - target function is usually discrete valued (ID3/C4.5)
    - disjunctive hypotheses may be required
    - possibly noisy training data
        - training data may contain errors
        - missing attribute values in the training data
- **ID3 algorithm**
    - performs a greedy search through the space of possible decision trees ⇒ local optimum instead of the global one

- recursive construction
  - select the “best” decision attribute for the current node
    - the attribute that is the most useful for classifying the examples
  - create descendants of the current node and build the subtrees recursively
- for selecting the “best” attribute the **information gain** (IG) measure is used
  - measures the expected reduction in **impurity** due to sorting on the attribute
  - measures for **impurity**
    - **entropy**



- S is a sample of training examples
- $p_\oplus$ is the proportion of positive examples in S
- $p_\ominus$ is the proportion of negative examples in S
- Entropy measures the impurity of S

$$Entropy(S) \equiv -p_\oplus \log_2 p_\oplus - p_\ominus \log_2 p_\ominus$$ [1]

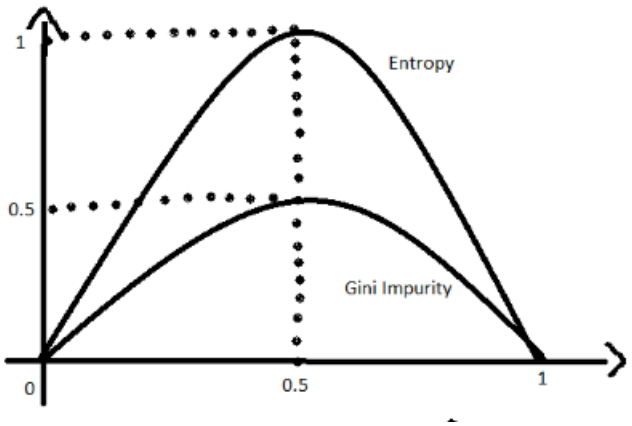
- c classes

$$E(S) = \sum_{i=1}^{c} -p_i log_2 p_i$$

$$Gain(S, A) \equiv Entropy(S) - \sum_{v \in Values(A)} \frac{|S_v|}{|S|} Entropy(S_v)$$

- **Gini index**

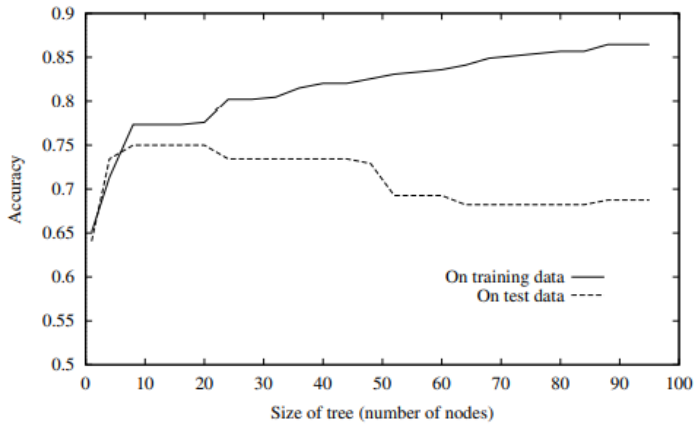
$$Gini = 1 - \sum_{i=1}^{n} (p_i)^2$$



- about the same performance using entropy and Gini index

- **Inductive bias in ID3**
  - preference for short trees, and for those with **high information** gain near the root
  - long hypotheses (trees) may be obtained by coincidence

- **Overfitting in DT learning**



[1]

- avoiding overfitting by **pruning**
  - stop growing the tree when data split is not statistically significant
    - use χ^2 test to decide, when building the DT, if pruning should be applied at a certain node
      - if the feature (attribute) at a certain node is uncorrelated with the decision of splitting the node, then prune
  - grow full tree, then post prune [1]
    - ***reduced error pruning***
      - use a validation set
      - evaluate the impact on the validation set of pruning each possible node (plus those below it)
    - ***rule post-pruning***
      - convert tree into rules
      - prune each rule independent of others

- more successful in practice
- used by C4.5

- **Issues in DT learning [1]** – handled by C4.5 algorithm
  - incorporating continuous valued attributes
  - alternative measures for selecting attributes
  - handling training examples with missing attribute values
  - handling attributes with costs

5. DT related research topics

- ensemble learning
  - Boosted Decision Trees
  - Random Forests (bagging)
- Fuzzy Decision Trees
- Lazy Decision Trees
- Hybrid models
  - DT + ANN (Artificial Neural Networks)
  - DT + SVM (Support Vector Machines)
  - DT + HMM (Hidden Markov Models)

[SLIDES]

- Inductive learning and decision tree learning (F. Leon) [2]
- DTs (T. Mitchell) [1]

[READING]

- Decision tree learning (T. Mitchell) [1]
- Decision trees (N. Nillson) [2]

Bibliography

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