BITS Pilani

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Introduction to Data Science

Module # 6 : Data Wrangling

IDS Course Team

BITS Pilani

The instructor is gratefully acknowledging the authors who made their course materials freely available online.

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Feature Engineering

- Feature Engineering is the process of selecting and extracting useful, predictive signals from data.
- The goal is to create a set of features that best represent the information contained in the data, producing a simpler model that generalizes well to future observations.

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Feature Creation

- Create new attributes that can capture important information in a dataset much more efficiently than the original attributes.
- Two general methodologies:
  - Feature Extraction
  - Feature Construction

Feature Extraction

- Mapping features to a new space
- Mostly rely on domain knowledge
  - Fourier Transform
  - Wavelet Transform
  - Scale-Invariant Feature Transform (SIFT) for images
  - Vector space transformation for text (TF-IDF)

Feature Construction

- Create dummy features
  - often used to convert categorical variable to into numerical variables.

Customer ID	Gender	Payment Method
C001	Female	Online banking
C002	Male	Online banking
C003	Female	Credit card
C004	Male	Debit Card

Customer ID	Gender	Online banking	Credit card	Debit Card
C001	Female	1	0	0
C002	Male	1	0	0
C003	Female	0	1	0
C004	Male	0	0	1

Feature Construction

- Create derived features
- Mostly rely on domain knowledge

Customer ID	Gender	Session Begin	Session End
C001	Female	15-06-2019 10:30	15-06-2019 11:15
C002	Male	13-06-2019 08:00	13-06-2019 08:03
C003	Female	02-06-2019 16:25	02-06-2019 18:35
C004	Male	01-06-2019 11:20	01-06-2019 13:00

Customer ID	Gender	Session Duration
C001	Female	45
C002	Male	3
C003	Female	125
C004	Male	100

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Curse of Dimensionality

- As dimensionality increases the number of data points required for a classification model also increase exponentially.

Hughes Phenomenon

For a fixed number of training samples(N) in the data set the performance of the models decreases as dimensionality increase.

- Reasons for this phenomenon:
  - Redundant Features – Carry same data in some other form.
  - Correlation between features – the presence of one feature influence the other.
  - Irrelevant Features - those that are simply unnecessary.

Impact of Dimensionality

- Distance measures become meaningless in higher dimensions.
- Use cosine similarity for high dimensional spaces.
- Impact of dimensionality on cosine similarity is lower as compared to the Euclidean distance.
- If the data is dense then it's impact will be high.
- If it is sparse then impact will be lower.

Reduce Dimensionality

- Feature Subset Selection
  - Filter Methods
  - Wrapper Methods
  - Embedded Methods
- Dimension Reduction
  - PCA

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Feature Subset Selection

Motivation

- Improving the prediction performance of the models.
- Reduction in the training time required to build model.
- Providing a better understanding of the underlying process that generated the data.

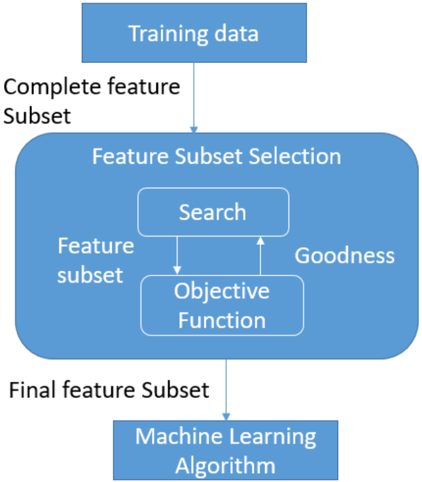
Feature Subset Selection

- Given: D initial set of features $F = \{f_1, f_2, f_3, \ldots, f_D\}$ and target class label T.
- Find: Minimum subset $F' = \{f'_1, f'_2, f'_3, \ldots, f'_M\}$ that achieves maximum classification performance where $F' \subseteq F$.
- There are 2^D possible subsets.
- Need a criteria to decide which subset is the best:
  - Classifier based on these M features has the lowest probability of error of all such classifiers.
- Evaluating 2^D possible subsets is time consuming and expensive.
- Use heuristics to reduce the search space.

Steps in Feature Selection

Feature selection is an optimization problem having the following steps:

- Step1: Search the space of all possible features.
- Step2: Pick the optimal subset using an objective function.



Feature Selection Approaches

- Unsupervised: Filter Methods
  - Use only features/predictor variables.
  - Select the features that have the most information.
- Supervised: Wrapper Methods
  - Train using the selected subset.
  - Estimate error on the validation set .
- Embedded Methods
  - Feature selection is done while training the model.
  - Example: Lasso (L1) Regularization and Decision Tree

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Filter Methods

- The Predictive power of individual feature is evaluated.
- Rank each feature according to some uni-variate metric and select the highest ranking features.
- Compute a score for each feature.
- The score should reflect the discriminative power of each feature.
- Advantages
  - Fast
  - Provides generically useful feature set.
- Disadvantages
  - Cause higher error than wrapper methods.
  - A feature that is not useful by itself can be very useful when combined with others. Filter methods can miss it.

Filter Methods

Algorithm

Given Input: large feature set F.

1. Identify candidate subset $S \subseteq F$.
2. While ! stop_ criterion()
   1. Evaluate utility function J using S.
   2. Adapt S.
3. Return S.

Types of Filters

- Correlation-based
  - Pearson product-moment correlation
  - Spear-man rank correlation
  - Kendall concordance
- Statistical/probabilistic independence metrics
  - Chi-square statistic
  - F-statistic
  - Welch's statistic
- Information-theoretic metrics
  - Mutual Information (Information Gain)
  - Gain Ratio
- Others
  - Fisher score
  - Gini index
  - Cramer's V

Which Filter ?

How do I pick the right filter ?

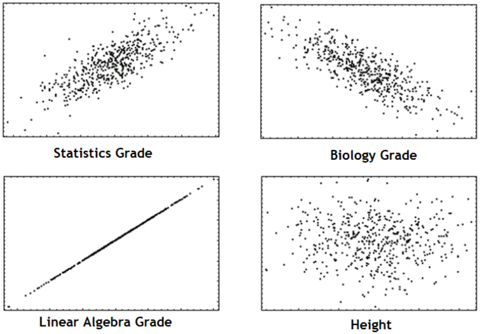
- Type of variables/targets (continuous, discrete, categorical).
- Class distribution
- Degree of non-linearity / feature interaction.

No Free Lunch Theorem

No Free Lunch theorem states that there is no universal model that works best for every problem.

Univariate filters

- How "useful" is a single feature?
- Correlated features are redundant.
- Keep the feature that has higher correlation.
- Predict the ML grade from the following features.



Pearson's Correlation Coefficient

- Used to measure the strength of association between two continuous features.
- Both positive and negative correlation are useful.

Steps

1. Compute the Pearson's Correlation Coefficient for each feature.
2. Sort according the score.
3. Retain the highest ranked features, discard the lowest ranked.

Limitation

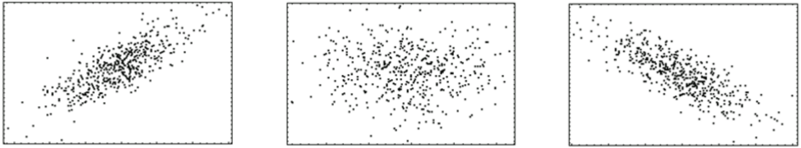
- Pearson assumes all features are independent.
- Pearson identifies only linear correlations

Pearson's Correlation Coefficient

$$\text{Feature: } x_k = \{x_k^{(1)}, \ldots, x_k^{(N)}\}^T$$

$$\text{Target: } y = \{y^{(1)}, \ldots, y^{(N)}\}^T$$

$$\rho(x, y) = \frac{\sum_{i=1}^{N} \left(x^{(i)} - \bar{x}\right)\left(y^{(i)} - \bar{y}\right)}{\sqrt{\left(x^{(i)} - \bar{x}\right)^2}\sqrt{\left(y^{(i)} - \bar{y}\right)^2}}$$



$r = +0.5$ $r = 0.0$ $r = -0.5$

Pearson's Correlation Coefficient

Check whether sale of ice creams and sun glasses are related?

Ice cream sale	Sun glasses sale
A	B
20	30
10	5
23	29
5	10

Pearson's Correlation Coefficient

A	B	$A - \bar{A}$	$(A - \bar{A})^2$	$B - \bar{B}$	$(B - \bar{B})^2$	$(A - \bar{A})(B - \bar{B})$
20	30	5.5	30.25	11.5	132.25	63.25
10	5	-4.5	20.25	-13.5	182.25	60.75
23	29	8.5	72.25	10.5	110.25	89.25
5	10	-9.5	90.25	-8.5	72.25	80.75
58	74		263		497	294

Pearson's Correlation Coefficient

$$\bar{A} = \frac{58}{4} = 14.5$$

$$\bar{B} = \frac{74}{4} = 18.5$$

$$\sigma_A = \sqrt{\frac{213}{3}} = 8.43$$

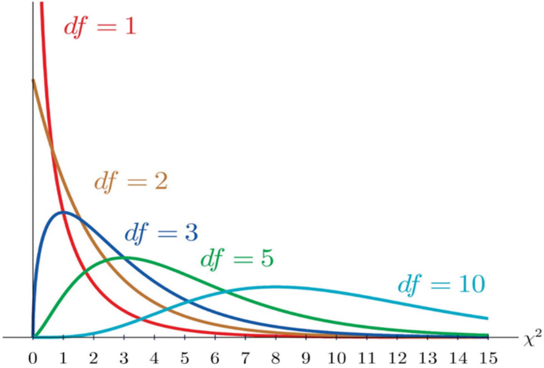
$$\sigma_B = \sqrt{\frac{497}{3}} = 12.87$$

$$r_{A,B} = \frac{294}{4 * 8.43 * 12.87} = 0.68 \approx 1$$

$$= \text{So positively correlated.}$$

χ^2 Statistic

- Chi-square test of independence allow us to see whether or not two categorical variables are related or not.
- The probability density function for the χ^2 distribution with r degrees of freedom (df) .



χ^2 Statistic

A group of customers were classified in terms of personality (introvert, extrovert or normal) and in terms of color preference (red, yellow or green) with the purpose of seeing whether there is an association (relationship) between personality and color preference.
Data was collected from 400 customers and presented in the $3(rows) \times 3(cols)$ contingency table below.

Observed Counts	Colors			
Personality	Red	Yellow	Green	Total
Introvert	11	5	1	17
Extrovert	8	6	8	22
Normal	3	10	12	25
Total	22	21	21	64

χ^2 Statistic

Step 1:

- Set up hypotheses and determine level of significance.
- Null hypothesis(H_0): Color preference is independent of personality.
- Alternative hypothesis(H_A): Color preference is dependent on personality .
- Level of significance: specifies the probability of error. Generally it is set as 5%.

$$\alpha = 0.005$$

- Assume that H_0 is always true unless the evidence portraits something else in which case we will reject H_0 and accept H_A.

χ^2 Statistic

Step 2:

- Compute the expected count.

$$E = \frac{\text{Row total} \times \text{Column total}}{\text{Grand total}}$$

Expected Counts	Colors			
Personality	Red	Yellow	Green	Total
Introvert	5.8	5.6	5.6	17
Extrovert	7.6	7.2	7.2	22
Normal	8.6	8.2	8.2	25
Total	22	21	21	64

χ^2 Statistic

Step 3:

- Compute the Chi-Squared Statistic.

$$\chi^2 = \sum \frac{(O - E)^2}{E}$$

- If H_0 is true, there should not be any difference between the observed values and expected values.

$$\chi^2 = \frac{(11 - 5.8)^2}{5.8} + \frac{(5 - 5.6)^2}{5.6} + \ldots + \frac{(12 - 8.2)^2}{8.2} = 14.5$$

χ^2 Statistic

Step 4:

- Use a probability table to find P-Value associated with χ^2 value for with degrees of freedom.

$$df = (r-1)(c-1)$$

  r is the number of categories in one variable and c is the number of categories in the other.

- $df = (3-1) \times (3-1) = 4$ (contingency table)

	Significance Level				
df	0.10	0.05	0.025	0.01	0.005
1	2.7055	3.8415	5.0239	6.6349	7.8794
2	4.6052	5.9915	7.3778	9.2104	10.5965
3	6.2514	7.8147	9.3484	11.3449	12.8381
4	7.7794	9.4877	11.1433	13.2767	14.8602
5	9.2363	11.0705	12.8325	15.0863	16.7496
6	10.6446	12.5916	14.4494	16.8119	18.5475
7	12.017	14.0671	16.0128	18.4753	20.2777

- $P(\chi^2 = 14.5) = 0.0058$ (from probability table)

χ^2 Statistic

Step 5:

$$
\begin{aligned}
\alpha &= 0.05 \\
P(\chi^2 = 14.5) &= 0.0058 \\
&< \alpha
\end{aligned}
$$

So reject H_0.
Accept H_A.
The two features are independent.

Information Theory Metrics

- Information-theoretic concepts can only be applied to discrete variables.
- For continuous feature values, some data discretization techniques are required beforehand.
- Three metrics
  - Information Gain
  - Gain Ratio
  - Gini Index

Information Gain

- Information Gain $IG(X, Y)$ is a measure of the mutual independence between two random variables X and Y.
- Measures non-linear dependencies.

$$IG(X, Y) = H(Y) - H(Y|X)$$
$$= \sum_{x_i \in X} \sum_{y_i \in Y} P(x_i, y_j) \frac{\log_2 P(x_i, y_j)}{P(x_i)P(y_j)}$$
$$IG(X, Y) = IG(Y, X)$$

- Information Gain is symmetric.
- Higher Information Gain; better prediction of Y given X.
- $I(X, Y) = 0$ if X and Y are independent.
- Biased towards the features having large number of discrete values.

Information Gain

Compute the Information Gain for the attribute Travel Cost wrt Transport Mode.

Gender	Car Ownership	Travel Cost	Income Level	Transport Mode
Male	0	Cheap	Low	Bus
Male	1	Cheap	Medium	Bus
Female	0	Cheap	Low	Bus
Male	1	Cheap	Medium	Bus
Female	1	Expensive	High	Car
Male	2	Expensive	Medium	Car
Female	2	Expensive	High	Car
Female	1	Cheap	Medium	Train
Male	0	Standard	Medium	Train
Female	1	Standard	Medium	Train

Information Gain

- Step 1: Compute the Entropy of target.

Transport Mode		
Bus	Car	Train
4	3	3

$$
\begin{aligned}
H(Transport) &= H(4,3,3) \\
&= -\frac{4}{10}\log_2\frac{4}{10} - \frac{3}{10}\log_2\frac{3}{10} - \frac{3}{10}\log_2\frac{3}{10} \\
&= 1.571
\end{aligned}
$$

Information Gain

- Step 2: Compute the Entropy of target given one feature.

Feature	Transport Mode		
	Bus	Car	Train
Cheap	4	1	0
Expensive	0	0	3
Standard	0	2	0

$$
\begin{aligned}
H(\mathit{Transport} | \mathit{Cost}) &= H(5,3,2) \\
&= -\frac{5}{10}\left(\frac{4}{5}\log_2\frac{4}{5} + \frac{1}{5}\log_2\frac{1}{5}\right) - \frac{3}{10}\left(\frac{3}{3}\log_2\frac{3}{3}\right) - \frac{2}{10}\left(\frac{2}{2}\log_2\frac{2}{2}\right) \\
&= 0.36
\end{aligned}
$$

Information Gain

- Step 3: Compute the information gain.

$$
\begin{aligned}
IG(Transport|Cost) &= H(4,3,3) - (H(5,3,2) \\
&= 1.571 - 0.36 \\
&= 1.211
\end{aligned}
$$

Gain Ratio

- Gain Ratio $GR(X, Y)$normalizes Information Gain $IG(X, Y)$.
- The information gain ratio is a variant of the mutual information.

$$GR(X, Y) = \frac{IG(A)}{H(A)}$$

- Reduces the bias toward attributes with many discrete values.
- The feature with the maximum gain ratio is selected as the best feature.

Gain Ratio

Compute the Gain Ratio for the attribute Travel Cost wrt Transport Mode.

Gender	Car Ownership	Travel Cost	Income Level	Transport Mode
Male	0	Cheap	Low	Bus
Male	1	Cheap	Medium	Bus
Female	0	Cheap	Low	Bus
Male	1	Cheap	Medium	Bus
Female	1	Expensive	High	Car
Male	2	Expensive	Medium	Car
Female	2	Expensive	High	Car
Female	1	Cheap	Medium	Train
Male	0	Standard	Medium	Train
Female	1	Standard	Medium	Train

innovate achieve lead

Gain Ratio

- Step 1: Compute the Entropy of target.

$$\begin{aligned} H(\mathit{Transport}) &= H(4,3,3) \\ &= -\frac{4}{10}\log_2\frac{4}{10} - \frac{3}{10}\log_2\frac{3}{10} - \frac{3}{10}\log_2\frac{3}{10} \\ &= 1.571 \end{aligned}$$

- Step 2: Compute the Entropy of feature.

$$\begin{aligned} H(\mathit{Cost}) &= H(5,3,2) \\ &= -\frac{5}{10}\log_2\frac{5}{10} - \frac{3}{10}\log_2\frac{3}{10} - \frac{2}{10}\log_2\frac{2}{10} \\ &= 1.48 \end{aligned}$$

Gain Ratio

- Step 3: Compute the Entropy of target given one feature.

$$
\begin{aligned}
H(\mathit{Transport} | \mathit{Cost}) &= H(5,3,2) \\
&= -\frac{5}{10}\left(\frac{4}{5}\log_2\frac{4}{5}+\frac{1}{5}\log_2\frac{1}{5}\right)-\frac{3}{10}\left(\frac{3}{3}\log_2\frac{3}{3}\right)-\frac{2}{10}\left(\frac{2}{2}\log_2\frac{2}{2}\right) \\
&= 0.36
\end{aligned}
$$

Gain Ratio

- Step 4: Compute the information gain.

$$\begin{aligned} IG(Transport|Cost) &= H(4,3,3) - (H(5,3,2) \\ &= 1.571 - 0.36 \\ &= 1.211 \end{aligned}$$

- Step 5: Compute Gain Ratio.

$$\begin{aligned} GR(Transport|Cost) &= \frac{IG(Transport|Cost)}{H(Cost)} \\ &= \frac{1.211}{1.48} \\ &= 0.818 \end{aligned}$$

Gini Index

- Gini index minimizes the probability of misclassification.
- Used in CART (Classification and Regression Tree) algorithms.

$$Gini = 1 - \sum_{i=1} Kp_k^2$$

where p_k denotes the proportion of instances belonging to class k.

- Higher Gini Index; better prediction of Y given X.

Gini Index

Compute the Gini Index for the feature Travel Cost wrt Transport Mode.

Gender	Car Ownership	Travel Cost	Income Level	Transport Mode
Male	0	Cheap	Low	Bus
Male	1	Cheap	Medium	Bus
Female	0	Cheap	Low	Bus
Male	1	Cheap	Medium	Bus
Female	1	Expensive	High	Car
Male	2	Expensive	Medium	Car
Female	2	Expensive	High	Car
Female	1	Cheap	Medium	Train
Male	0	Standard	Medium	Train
Female	1	Standard	Medium	Train

Gini Index

- Step 1: Compute the Gini Index for each value of the feature.

$$Gini(Transport|Cost = Cheap) = 1 - (0.8^2 + 0.2^2) = 0.32$$

$$Gini(Transport|Cost = Expensive) = 1 - (1^2 + 0) = 0$$

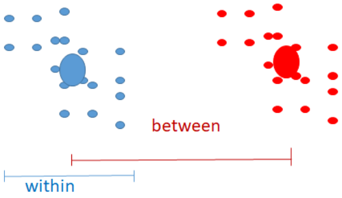
$$Gini(Transport|Cost = Standard) = 1 - (1^2 + 0) = 0$$

- Step 2: Compute the Gini Index for feature.

$$Gini(Transport|Cost) = \frac{5}{10} * 0.32 + \frac{3}{10} * 0 + \frac{2}{10} * 0 = 0.16$$

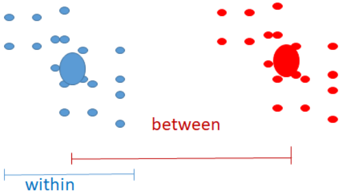
Fisher Score

- Applicable for classification problems with numeric features.
- Metrics can be applied naturally to real-valued features in a binary classification problem or multi-class classification problem.
- Between-class distance -– Distance between the centroids of different classes.
- Within-class distance -– Accumulated distance of an instance to the centroid of its class.



Fisher Score

- Fisher score is the measure the ratio of the average inter-class separation to the average intraclass separation.
- The larger the Fisher score, the greater the discriminatory power of the attribute.
- This score is often referred as signal to noise ratio.



Fisher Score

- The Fisher Ratio is defined as the ratio of the variance of the between classes to the variance of within classes.
- Fisher's ratio is a measure for (linear) discriminating power of a variable.
  - Maximum between class variance (difference of means).
  - Minimum within class variance (sum of variances).

$$F = \frac{\sum_{j=1}^{k} p_j(\mu_j - \mu)^2}{\sum_{j=1}^{k} p_j \sigma_j^2}$$

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Wrapper Methods

- Greedy Based algorithms.
- Performance of the method depends on the machine learning models chosen.
- Sequential feature selection algorithm add or remove one feature at a time based on the classifier performance until a desired criterion is met.
- Two methods
  - Sequential Forward Selection(SFS)
  - Sequential Backward Selection(SBS)
- Advantages
  - Highest performance
- Disadvantages
  - Computationally expensive
  - Memory intensive

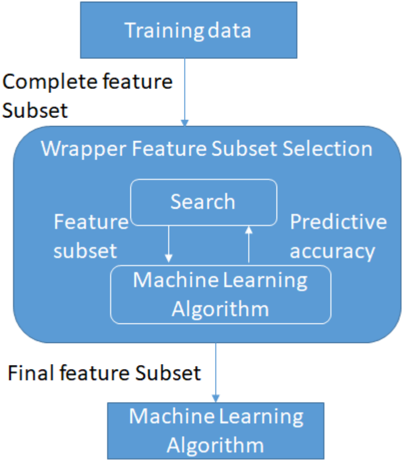
Wrapper Methods

Algorithm

Given Input: large feature set F.

1. Identify candidate subset $S \subseteq F$.
2. While ! stop_ criterion()
    1. Evaluate error of a classifier using S.
    2. Adapt subset S.
3. Return S.

- Commonly used stop criterion
    - Increase / Decrease in Predictive accuracy
    - Predefined number of features is reached



Sequential Forward Selection

Algorithm

1. Start with the empty set.

$$Y_0 = \{\Phi\}$$

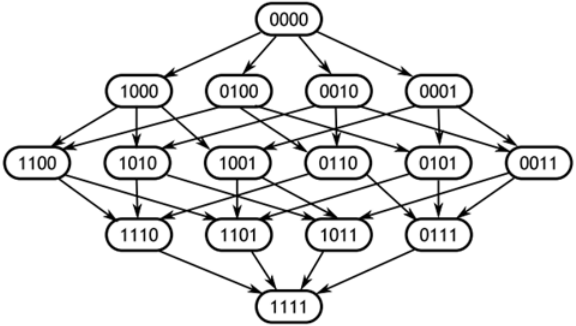
2. Add the next best feature.

$$x^* = argmax_{x \notin Y_k} \quad J(Y_k + x)$$

3. Update

$$Y_{k+1} = Y_k + x^* \qquad k = k + 1$$

4. Go to step 2.



Sequential Backward Selection

Algorithm

1. Start with the empty set.

$$Y_0 = X$$

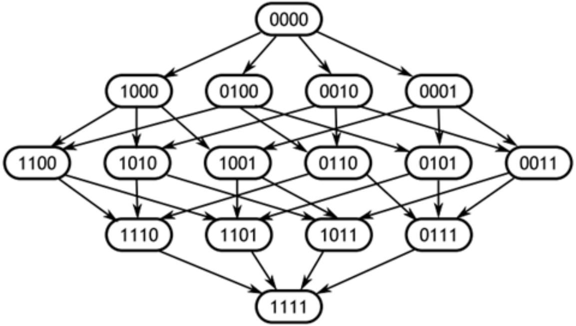
2. Remove the next worst feature.

$$x^* = argmax_{x \notin Y_k} \quad J(Y_k - x)$$

3. Update

$$Y_{k+1} = Y_k - x^* \qquad k = k + 1$$

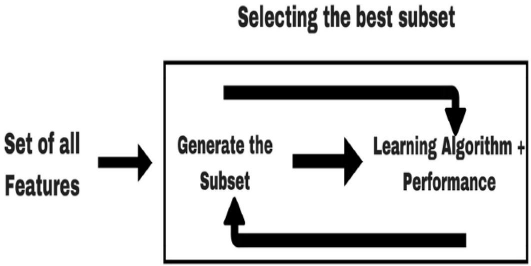
4. Go to step 2.



Backwards selection is frequently used with random forest models.

Embedded Methods

- Embedded methods combine the qualities of filter and wrapper methods.
- Implemented by algorithms that have their own built-in feature selection methods.



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Embedded Methods

- Some of the most popular examples of these methods are LASSO and RIDGE regression which have inbuilt penalization functions to reduce overfitting.
- Lasso regression performs L1 regularization which adds penalty equivalent to absolute value of the magnitude of coefficients.
- Ridge regression performs L2 regularization which adds penalty equivalent to square of the magnitude of coefficients.
- Regularized trees, Memetic algorithm, Random multinomial logit are also examples of Embedded Method.

Data Science - Concepts and Practice by Vijay Kotuand BalaDeshpande

- Introduction to Data Mining, by Tan, Steinbach and Vipin Kumar (T3)
- The Art of Data Science by Roger D Peng and Elizabeth Matsui (R1)
- Introducing Data Science by Cielen, Meysman and Ali
- Data Science - Concepts and Practice by Vijay Kotuand BalaDeshpande
- Data mining: Concepts and techniques, by Han, J., Kamber, M., and Pei, J. (2012). (3rd ed.)

THANK YOU