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## *Research Papers*

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# QSAR: MODERN TOOL OF DRUG DESIGN

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## ABSTRACT
*The application of quantitative structure–activity relationships (QSARs) has significantly revolutionised the whole process of drug discovery. QSAR models eases out the calculation of physicochemical properties (e.g., lipophobicity), the prediction of biological activity (or toxicity) of the potential drug molecule. It also predicts very well the absorption, distribution, metabolism, and excretion (ADME). QSAR has the most significant application in the preclinical stages of the drug discovery as this stage involves tedious work with high cost of experimentation. QSAR narrow downs and filter large chemical databases, and select suitable drug candidates. This article presents some current challenges and applications for the discovery and optimization of drug candidates based on QSAR methodology.*

*Keywords: QSAR, Drug design, New chemical entities (NCEs), ADME.*

## INTRODUCTION
Discovery and development of a new drug is an expensive and time consuming process. The therapeutic effects and hazards of the discovered drugs to health are assessed by *in-vivo* tests and by various experimental techniques. However, involvement of animal models raises ethical questions. Therefore, alternative methods are being developed to for drug testing. *In-silico* methods offers alternative path due to their lower cost. They offer significant contribution to the identification and development of effective drugs from new chemical entities (NCEs). The computational tools are principally used for

- Conformational analysis of molecular structure (e.g., molecular dynamics)
- Characterization of drug–target interactions (e.g., molecular docking); and
- Assessment and optimization of drug activity using quantitative structure-activity relationships (QSARs).

QSAR methods are useful evaluating physicochemical features, physico-chemical properties and biological effects which govern a biological response in drug design. As a result, QSAR has emerged as low-cost tool filtering out novel "hits" and for "lead" optimization which is important process of drug discovery and development. The foundation of modern QSAR was laid by Prof. Corwin Hansch and co-workers during the early 1960s[1]. Since then, various QSAR models have come into existence for understanding of biological and physicochemical properties of NCEs and their evaluation. This emergence of QSAR for design and development of new drugs is evident by the cascade of publications and QSAR-based software. The aim of this article is to signify the application of QSAR in drug design.

## PRECLINICAL PHASES: FROM NEW CHEMICAL ENTITIES (NCES) TO DRUG CANDIDATES
To ensure the therapeutic effect and the safety of the new chemical entities (NCEs), the benefits (therapeutic effects) and the risk (toxic effects) of the NCEs are evaluated, respectively, during the preclinical and the clinical phases of development[2,3]. For a particular disease state once the target has been validated, relevant data is gathered in the preclinical drug development in order to propose a drug candidate for clinical test. Using *in-silico, in-vitro methods* and animal models, the pharmacological profile and the acute toxicity of the drug candidate are assessed during the preclinical stage. Figure 1 present the three-stage procedure allowing the selection of the most effective NCEs (the drug candidates).

### Stage 1: Hit idetification
This stage aims to identify "hit" compounds from diverse libraries (corporate, commercial, etc.) and/or by medical observations for a given target (receptor, enzyme, etc.). Various techniques like high-throughput screening (HTS) and *in-silico* evaluations are used to screen NCEs with suitable pharmacodynamic (PD) activity. The PD properties of a given molecular entity are defined as the physiological and biochemical effects of the entity on the body.

### Stage 2: Lead identification
This stage is a key milestone of the drug candidate discovery process. The pharmacokinetic (PK) properties govern the bioavailability of the NCEs and, therefore, the correct delivery of the drug to its target site. The PK properties are represented by the processes of absorption, distribution, metabolism, and elimination (ADME) under-gone by the NCEs in the organism. During this stage, "hit" molecules presenting good ADME and physicochemical properties are identified and taken further as lead compounds.

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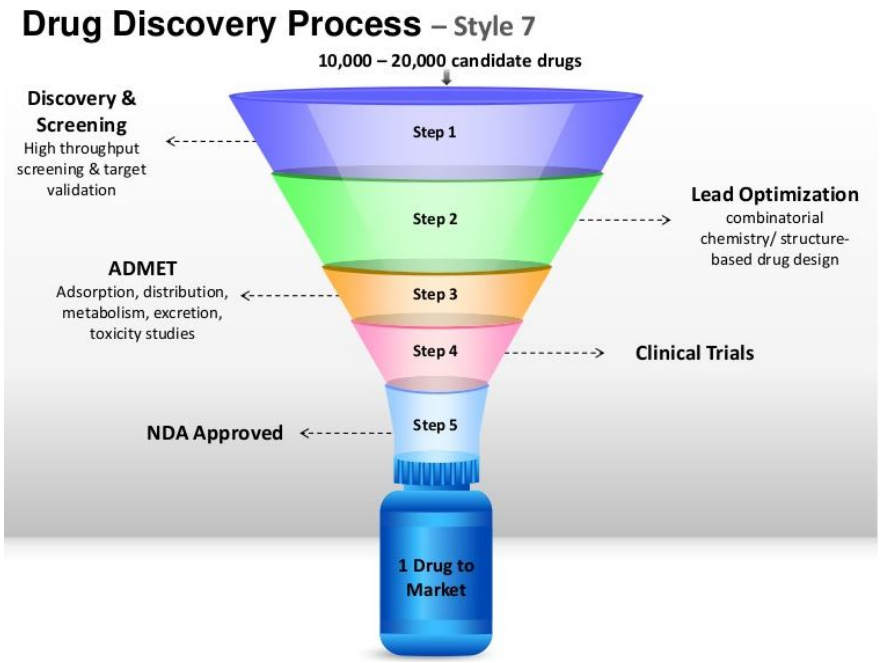


**Figure 1: Strategy for a validated pharmaceutical target. Drug candidates are selected following various stages of development: (1) the selection of "hit" compounds, (2) the optimization of "lead" compounds, and (3-5) the choice of the drug candidates**

**Stage 3: Lead Optimization**

This stage involves the evaluation of various properties of lead analogs in order to propose the drug candidates. Accordingly, lead's molecular scaffold is modified to generate lead analogs. Then the drug candidates are selected based on the chemical structures with the optimal potency, solubility, and ADME profile. QSAR and molecular docking have a major role to play in selecting strategies for lead finding and optimization. Once the preclinical phase is complete, the selected drug candidates can be subjected to phases I, II, and III of clinical development.

**DRUG DISCOVERY PROCESS: A TIME CONSUMING PROCESS**

Simple rules of thumb, such as the "rule of 5" (also known as Lipinski's rules can be used to filter molecules which are likely to be only weakly bio available. However, experimental evaluation can be time consuming, expensive, or be subject to ethical barriers. In this context, QSAR methods analyses allow the identification of the structural and physicochemical features modulating the activities of compounds.

Thus QSAR method by passes the cumbersome process of laboratory work of optimizing the drug candidate directly gives the potential drug molecules for the preclinical analysis. Figure 2 represents the time involved in the drug discovery process and impact of QSAR in drug design.

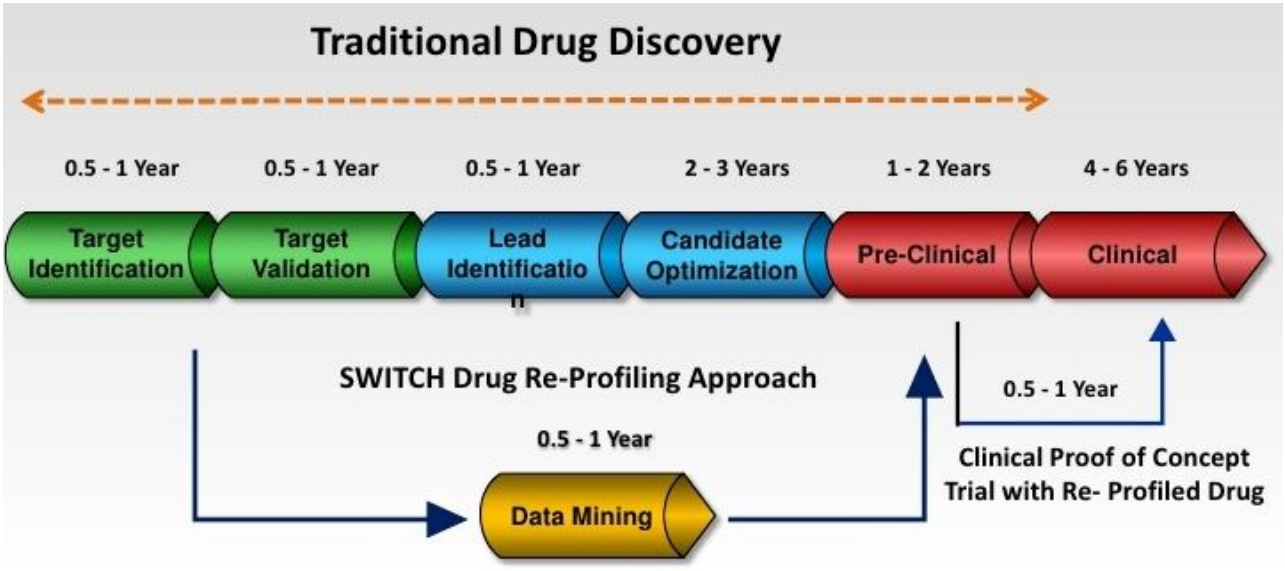


**Fig2: Impact of QSAR methodology in drug design and discovery process.**

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## REASONS FOR FAILURE IN DRUG CANDIDATE DEVELOPMENT

The development of a typical drug may cost up to one billion US dollars and 10-15 years of time. Even though after applying stringent procedure and substantial financial investment of drug development tested in the preclinical phase, out of 5000 molecules, only one reaches the market[4]. Kennedy et al.[5] have studied the factors which cause failures during clinical assessments (Figure 3). Insufficient pharmacokinetic properties (39%), lack of efficacy (30%), toxicity in animals (11%), and adverse effects to man (10%) are the major reasons to explain the exit of molecules in pharmaceutical research. Poor ADME properties are major cause of failure during drug development[6,7].

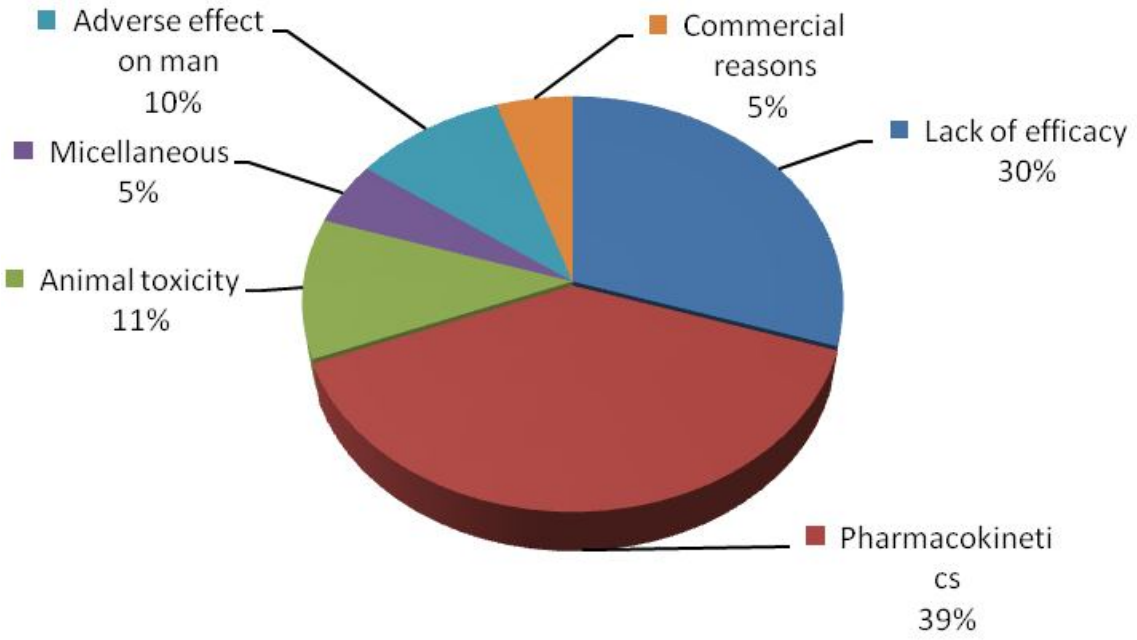


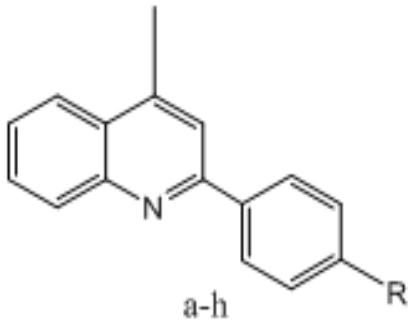

**Figure 3: Reasons for the failure of the development of NCEs in clinical development[5]**

To address ADME and potency during the early phase of drug discovery and development, numerous computational tools, have been proposed[8–10].These tools vary from very trivial "rules of thumb," e.g., Lipinski's rule of 5[11] to more complex and multivariate QSAR models, which includes the use of models based on neural networks[12,13].

## QSAR PROCESS

### DEVELOPMENT OF TRAINING AND TEST SET

The first step in deriving a QSAR model is to gather and select the molecules with activity data to include in the training set and test set. The resulting information can be downloaded in different formats (e.g., SMILES, sdf file, txt file). Using the QSAR methods, Chourasia et al[14] designed and evaluated a series of 4-methyl-2-(p-substitutedphenyl) quinoline derivatives as potential antifungal agents. The general structure of the synthesized quinoline derivatives is shown in figure 4.




R= -H,-$CH_3$,-$OCH_3$,-OH,-$NO_2$,-Cl,-Br,-COOH

**Fig 4: Structure of the synthesized test set quinoline derivatives**

Various physicochemical descriptors like constitutional, molecular, steric, and electronic were calculated by the Datawarrier[15] Software .The descriptors used to develop the model are listed and described in the Table 2.

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*Table 2. Descriptors used for the training and test set*

| S. No. | Descriptor used | Symbol |
|---|---|---|
| 1 | Total Molweight in g/mol; natural abundance | **TMW** |
| 2 | cLogP; P; conc(octanol) /conc(water) | **cLogP** |
| 3 | Total surface area(from polar and non-polar SAS Approximation) | **TSA** |
| 4 | Druglikeness | **Drug** |
| 5 | Lipophilic Ligand Efficiancy (LLE) | **LLE** |
| 6 | Ligand Efficiency Lipophilic Price(LELP) | **LELP** |
| 7 | Molecular shape Index | **MSI** |
| 8 | Rotatable Bond Count | **RBC** |

**REGRESSION ANALYSIS**

Using the calculated descriptors multiple linear regressions were performed using the software SPSS[16] by stepwise method. The best model derived from the regression analysis was used to predict the biological activity of the synthesised compounds. No outliers have been determined and the equations were derived using the entire training data set (n=30). The summary of the model generated is given in the Table 3.

*Table 3. Summary of the QSAR model generated by the regression analysis*

*Model Summary*

| Model | R | R Square | Adjusted R Square | Std. Error of the Estimate | Durbin-Watson |
|---|---|---|---|---|---|
| 1 | 0.762 | 0.580 | 0.420 | 0.9830729 | 2.296 |

Predictors: (Constant), Rotatable_Bonds, Total_Surface_Area, Druglikeness, Shape_Index, Total_Molweight, LLE, cLogP, LELP

Dependent Variable: Reported activity

**VALIDATION TEST**

The equations 1 and 2 are generated by the model. The equations, then, were used to calculate the unknown activities of the test set compounds.

**QSAR model for A. Niger**

Biological activity (ZOI) = (18.354)+ (-0.007* **TMW**)+ (4.359***cLogP**)+( 0.132* **TSA**)+ (0.315*Drug)+ (2.963***MSI**)+ (-0.419***RBC**) -------- eq. (1)

**QSAR model for C. Albicans**

Biological activity (ZOI) = (18.354)+ (-0.007* **TMW**)+ (4.359***cLogP**)+( 0.132***TSA**)+ (0.315*Drug)+ (2.963* **MSI**)+ (-0.419***RBC**) --------- eq. (2)

Using the equations, the predicted antifungal activities of the synthesized test set quinoline compounds were calculated. This gave the predicted antifungal activity of the test set compound with unknown activity. Had conventional method of synthesis and determination of the antifungal activity being applied, it would cost money and time for the same pocess.

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## IN-VITRO ANTIMICROBIAL ACTIVITY

Once the QSAR predicted activity of the test set quinoline compounds are determined, the model has to be validated by comparing the predicted activities with the experimental ones. For this standard method were applied and the *in-vitro* antifungal activities of the synthesized test set quinoline compounds were determined. Figure 5 gives a comparative account of the predicted and experimental activities.

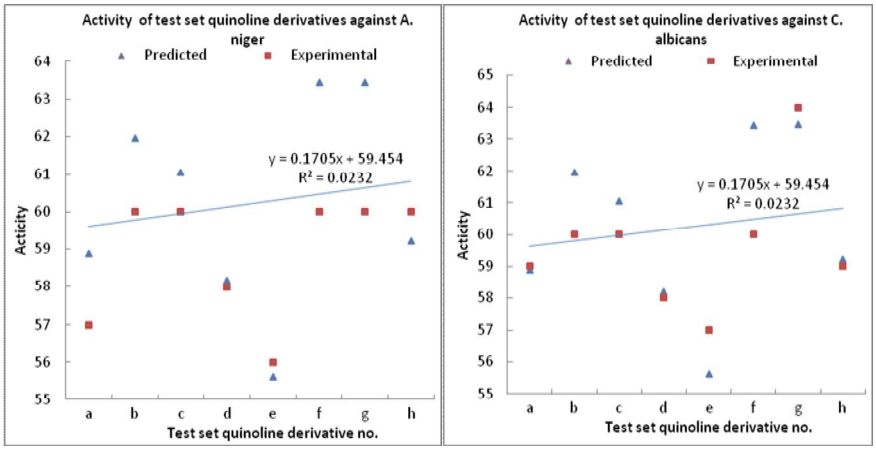


**Fig. 5: Comparison of predicted and experimental antifungal activities of the synthesized test set quinoline compounds**

A set of 8 quinoline compounds were developed and a comparative study of the predicted and experimental activities was made. It is clear from the graph that the *in-vitro* antifungal activities are close the predicted activities. This itself validates the generated QSAR model

## RESULT AND DISCUSSION

The predicted and experimental antifungal activity for the synthesized test set quinoline compounds have been found in good agreement. A low value of $R^2$ suggest that the descriptor used for the model are significant and show little co-relation with one another. This validated the generated QSAR model and hence it can be used to predict the antifungal activities of the other quinoline derivatives with unknown biological activity.

## CONCLUSION

The generated QSAR model in this case offers an alternative quick and economic path for the pre-clinical phase i.e. target validation, lead identification and lead optimization in the drug discovery process.

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# INFORMATION TECHNOLOGY IN DATA SCIENCE

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**ABSTRACT**
*The most successful person is the one who has the best information and the ability to apply it effectively. This remark summarizes the business of information technologies in the context of generation, storage, processing and use of information. Today, cutting-edge technologies such as computers, software and artificial intelligence, fiber optics and networking have an immense impact on information technology. Among the many applications of information technology, three of particular importances are traditional telephony, mobile cellular telephony, and data processing and communication. Advancement in information technology, affect many industries and society as a whole.*

*This research article discusses the effect of advanced computer science and information technology in the context of data science.*

*Keywords: E-Commerce, Data Science, Machine Learning, Data Analytics, SAS, SQL, Python, Exploratory Data Analysis, Confirmatory Data Analysis.*

## I. INTRODUCTION

In the past few decades there has been great revolution in computing and communication technology. One can book a movie ticket, shop online, transfer money via different commercial websites on a single click. Such a progressed transformation is due to advances in handy devices, digital media and geo-based technology. Such multi-channel shopping revolution has put the customer in control, convincing the retailers to look for a single, seamless approach that lets them interact with their customers anytime and anywhere, across any and all channels. E-commerce companies have now turned to Data Science for focused customer group targeting and evaluating campaign strategies., E-commerce companies are greatly using data science to push the customers to the wide range of products & sell it as per customer's purchasing power and concern. Use of Data Science plays an important role in tracking the entire journey of a customer, from entry to exit on a particular commercial website. An average online shopper may not realise that every click is being monitored and that all purchases being made are captured from beginning to end. Due to this the customers get easily divided into different sectors based on the combination of their purchase patterns and demographic details . This not only provides an interactive and richer experience to customers, but also improves the retailer's ability to increase sales through cross-sell and up-sell.

## II. WHAT IS DATA SCIENCE?

Data science, also known as data-driven science, is an interdisciplinary field about scientific methods, processes, and systems to extract knowledge or insights from data in various forms, either structured or unstructured. Data science is a "concept to unify statistics, data analysis and their related methods" in order to "understand and analyze actual phenomena with data". It employs techniques and theories drawn from many fields within the broad areas of Mathematics, Statistics, Information Science and Computer Science.

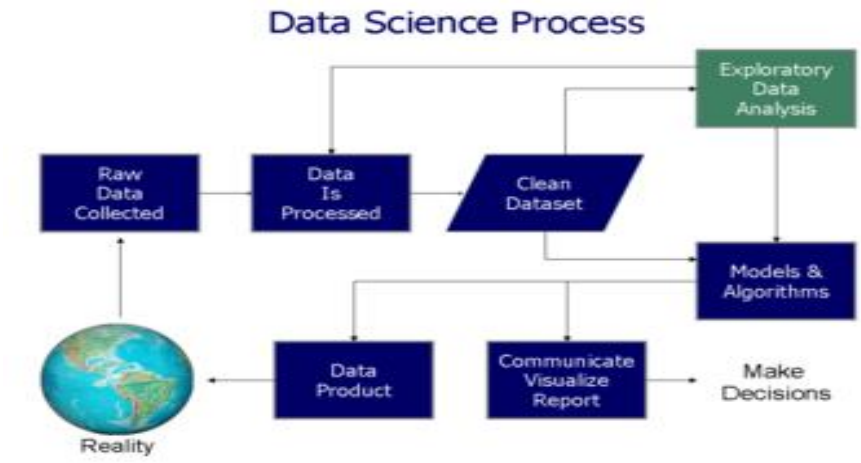


Fig.1: Data science process flowchart -"Doing Data Science", Cathy O'Neil and Rachel Schutt, 2013

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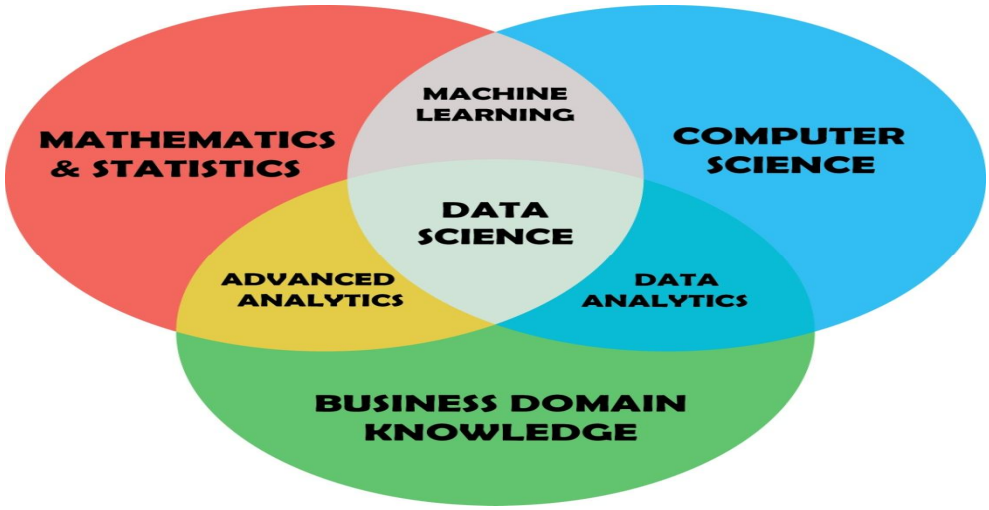


Fig. 2 : Data Science as in Venn Diagram

The above venn diagram elaborates Data Science as the combination of fields such as Computer Science, Mathematics and Statistics .The domain knowledge about the particular business also plays vital role in Data Science. Machine learning and Data Analytics are the blends of aforesaid fields.

**• Machine Learning**

The term machine learning means the automatic detection of significant patterns in data. Since last couple of years it has become a common implement in almost any task that requires essence of information gathered from large data sets. The search engines like Google, Yahoo are nothing but machine learning based technologies which are used to bring us the best results by placing worthwhile advertisements. The anti-virus software are also machine learning based technologies which filter our email messages, credit card transactions are secured by a software that learns how to detect frauds. Digital cameras learn to detect faces and voice commands given by us are recognized by intelligent personal assistance applications on smart-phones . The accident prevention systems in cars are built using machine learning algorithms. Machine learning is also widely used in scientific applications such as bioinformatics, medicine, and astronomy. Thus Machine Learning tools give us programs with the ability to "learn" and adapt.

**• Data Analytics**

Data Analytics is the science of inspecting raw data with the purpose of locating patterns and drawing inferences about the information by applying an algorithmic or mechanical process to derive insights. Data analytics methodologies consists of two types of techniques :

i) Exploratory Data Analysis (EDA) - It is applied to find patterns and relationships in data.

ii) Confirmatory Data Analysis (CDA)- It involves use of various statistical techniques to determine whether the claims stated about a data set are proper or not.

An eminent statistician John W. Tukey says- "EDA is often compared to detective work, while CDA is akin to the work of a judge or jury during a court trial"

## III. APPLICATIONS OF DATA SCIENCE

**• Web browsing**

The web search engines like Google, Yahoo, AOL, Ask, Bing etc. deliver the best results for our online search queries in fraction of seconds using the data science algorithms.

**• Targeted Digital Advertisements**

Traditional advertising is now well complimented by the Digital advertising / marketing field due to effective use of Data Science. Display banners & advertisements on various websites and social media sites, digital bill boards at airports, are decided by use of data science. This has significantly helped to increase Click Through Rate (CTR) of digital advertisements. This is the reason why one sees ads of job/ immigration opportunities while his/her friend sees ad of kitchenware products in the same place at the same time.

**• Recommender Systems**

A lot of companies like Amazon, Twitter, Google Play, Netflix, LinkedIn have aggressively used this system to promote their products / suggestions in accordance with user's interest and relevance of information. The recommendations are made based on previous search results of a user.

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• **Image Recognition**
Social media websites automatically helps to tag your friends when you upload your photos there. Such tagging is done using Image Recognition .It also gives you a suggestion to connect & find new friends through mutual networks. This automatic tag suggestion feature uses face recognition algorithm. Similarly, while paying or transferring money, one can scan a barcode or QR code in web browser using mobile phone. It uses image recognition.

• **Airline Route Planning**
Airline Industry across the world is known to have heavy losses which are attributed to various reasons. Maintaining occupancy ratio and operating profits. High fluctuation in air fuel prices and need to offer heavy discounts to customers have further made the situation worse. Use of data science has tactically provided the solution and areas of improvements. Now using data science, the airline companies can predict flight delay, decide which class of airplanes to buy, whether to directly land at the destination, or take a halt in between, decide the air fares based on passenger density on a given route and effectively drive customer loyalty programs etc.

• **Fraud and Risk Detection**
Data Science is also applied in Finance sector. Finance companies were losing their profits because of amount overdue by customers and losses every year. However, they had a lot of data which were collected during the initial paper work while sanctioning loans. They decided to practise data science in order to liberate them out of losses. Hence banking companies learned how to collect the data via customer profiling, their past expenditures and other essential variables to analyze the probabilities of risk and default. Moreover, it also helped them to push their banking products based on customer's purchasing power.

Apart from the applications mentioned above, data science is also used in Marketing, Finance, Human Resources, Health Care, Government Policies and every possible industry where data gets generated. Using data science, the marketing departments of companies decide which products are best for Up selling and Cross selling, based on the data related to customer's choice. In addition, predicting the wallet share of a customer, which customer is likely to churn, which customer should be kicked for high value product and many other questions can be easily answered by data science. Finance (Credit Risk, Fraud), Human Resources (which employees are most likely to leave, employees performance, decide employees bonus) and many other tasks are easily accomplished using data science in these disciplines.

## IV. SKILL SET AND SCOPE FOR BEING A DATA SCIENTIST

Data Scientist have a huge scope in India, for experienced as well as fresher who want to make a career in data science. These are some of the top Indian companies that hire data scientists –

**Service-based company –**
Fractal Analytics, Mu Sigma, Citi, HCL, Uber, Goldman Sachs, IBM, CapGemini , Accenture.

**Product-based company**- Amazon, Flipkart, Paytm, Haptik etc.

The skills needed to be data scientists:

- In-depth knowledge of SAS and/or R. For Data Science, R is generally preferred.
- Python coding: Python is the most common coding language that is used in data science along with Java, Perl, C/C++.
- SQL database/coding: Preferred candidates can write and execute complex queries in SQL.
- Working with unstructured data: It is extremely important that a Data Scientist is able to work with unstructured data—whether from social media, video feeds, audio or other sources.

## V. CONCLUSION

Today, developments in Information Technology have changed the socio-economic status of the society in terms of flexibility in computing, communication and business. It has generated n number of job opportunities in the fields of computer science as well as E-Commerce. People with exact domain knowledge and proper skill set regarding a particular job profile gets absorbed immediately with impressive salary structure. This indicates a positive sign to the growth of Indian Economy.

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6. https://www.searchdatamanagement.techtarget.com/
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## EXAMPLES OF REFERENCES

All references must be arranged first alphabetically and then it may be further sorted chronologically also.

- **Single author journal article:**

Fox, S. (1984). Empowerment as a catalyst for change: an example for the food industry. *Supply Chain Management*, *2*(3), 29–33.

Bateson, C. D.,(2006), 'Doing Business after the Fall: The Virtue of Moral Hypocrisy', Journal of Business Ethics, 66: 321 – 335

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Khan, M. R., Islam, A. F. M. M., & Das, D. (1886). A Factor Analytic Study on the Validity of a Union Commitment Scale. *Journal of Applied Psychology*, *12*(1), 129-136.

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Simchi-Levi, D., Kaminsky, P., & Simchi-Levi, E. (2007). *Designing and Managing the Supply Chain: Concepts, Strategies and Case Studies* (3rd ed.). New York: McGraw-Hill.

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- **Electronic sources should include the URL of the website at which they may be found, as shown:**

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- **Unpublished dissertation/ paper:**

Uddin, K. (2000). A Study of Corporate Governance in a Developing Country: A Case of Bangladesh (Unpublished Dissertation). Lingnan University, Hong Kong.

- **Article in newspaper:**

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- **Article in magazine:**

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7. The submission implies that the work has not been published earlier elsewhere and is not under consideration to be published anywhere else if selected for publication in the journal of Indian Academicians and Researchers Association.

8. Decision of the Editorial Board regarding selection/rejection of the articles will be final.