Hui Lin and Ming Li

Introduction to Data Science

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Preface

During the first couple years of our career as data scientists, we were bewildered by all kinds of data science hype. There is a lack of definition of many basic terminologies such as “Big Data” and “Data Science.” How big is big? If someone ran into you asked what data science was all about, what would you tell them? What is the difference between the sexy role “Data Scientist” and the traditional “Data Analyst”? How suddenly came all kinds of machine algorithms? All those struck us as confusing and vague as real-world data scientists! But we always felt that there was something real there. After applying data science for many years, we explored it more and had a much better idea about data science. And this book is our endeavor to make data science to a more legitimate field.

Goal of the Book

This is an introductory book to data science with a specific focus on the application. Data Science is a cross-disciplinary subject involving hands-on experience and business problem-solving exposures. The majority of existing introduction books on data science are about the modeling techniques and the implementation of models using R or Python. However, they fail to introduce data science in a context of the industrial environment. Moreover, a crucial part, the art of data science in practice, is often missing. This book intends to fill the gap.

Some key features of this book are as follows:

- It is comprehensive. It covers not only technical skills but also soft skills and big data environment in the industry.

- It is hands-on. We provide the data and repeatable R and Python code. You can repeat the analysis in the book using the data and code provided. We also suggest you perform the analyses with your data whenever possible. You can only learn data science by doing it!
- It is based on context. We put methods in the context of industrial data science questions.
- Where appropriate, we point you to more advanced materials on models to dive deeper

Who This Book Is For

Non-mathematical readers will appreciate the emphasis on problem-solving with real data across a wide variety of applications and the reproducibility of the companion R and python code.

Readers should know basic statistical ideas, such as correlation and linear regression analysis. While the text is biased against complex equations, a mathematical background is needed for advanced topics.

What This Book Covers

Based on industry experience, this book outlines the real world scenario and points out pitfalls data science practitioners should avoid. It also covers big data cloud platform and the art of data science such as soft skills. We use R as the main tool and provide code for both R and Python.

Conventions

Acknowledgements

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Introduction

Interest in data science is at an all-time high and has exploded in popularity in the last couple of years. Data scientists today are from various backgrounds. If someone ran into you asked what data science was all about, what would you tell them? It is not easy to answer. Data science is one of the areas where you ask ten people who will give ten different answers. It is not well-defined as an academic subject but broadly used in the industry. Media has been hyping about "Data Science" "Big Data" and "Artificial Intelligence" over the fast few years. With the data science hype picking up stream, many professionals changed their titles to "Data Scientist" without any of the necessary qualifications. Your first reaction to all of this might be some combination of skepticism and confusion. We want to address this up front that: we had that exact reaction. To make things clear, let's start with the fundamental question.

1.1 What is data science?

David Donoho (Donoho, 2015) summarizes in "50 Years of Data Science" the main recurring "Memes" about data sciences:

1. The 'Big Data' Meme
2. The 'Skills' Meme
3. The 'Jobs' Meme

Everyone should have heard about big data. Data science trainees now need the skills to cope with such big data sets. What are those skills? You may hear about: Hadoop, a system using Map/Reduce to process large data sets distributed across a cluster of computers. The new skills are for dealing with organizational artifacts of large-scale cluster computing but not for better solving the real problem. A lot of data on its own is worthless. It isn't the size of the data that's important. It's what you do with it. The big data skills that so many are touting today are not skills for better solving the real problem of inference from data.

We are transiting to universal connectivity with a deluge of data filling telecom servers. But these facts don't immediately create a science. The statisticians and computer scientists have been laying the groundwork for data science for at least 50 years. Today's data science is an enlargement and combination of statistics and computer science rather than a brand new discipline.

Data Science doesn't come out of the blue. Its predecessor is data analysis. Back in 1962, John Tukey wrote in "The Future of Data Analysis":

> For a long time I have thought I was a statistician, interested in inferences from the particular to the general. But as I have watched mathematical statistics evolve, I have had cause to wonder and to doubt. ...All in all, I have come to feel that my central interest is in data analysis, which I take to include, among other things: procedures for analyzing data, techniques for interpreting the results of such procedures, ways of planning the gathering of data to make its analysis easier, more precise or more accurate, and all the machinery and results of (mathematical) statistics which apply to analyzing data.

It deeply shocked his academic readers. Aren't you supposed to present something mathematically precise, such as definitions, theorems, and proofs? If we use one sentence to summarize what John said, it is:

> data analysis is more than mathematics.

In September 2015, the University of Michigan made plans to invest $100 million over the next five years in a new Data Science Initiative (DSI) that will enhance opportunities for student and faculty researchers across the university to tap into the enormous potential of big data. How does DSI define Data science? Their website gives us an idea:

> "This coupling of scientific discovery and practice involves the collection, management, processing, analysis, visualization, and interpretation of vast amounts of heterogeneous data associated with a diverse array of scientific, translational, and interdisciplinary applications."

How about data scientist? Here is a list of somewhat whimsical definitions for a "data scientist":

- "A data scientist is a data analyst who lives in California"
- "A data scientist is someone who is better at statistics than any software engineer and better at software engineering than any statistician."
- "A data scientist is a statistician who lives in San Francisco."
- "Data Science is statistics on a Mac."

There is lots of confusion between Data Scientist, Statistician, Business/Financial/Risk(etc.) Analyst and BI professional due to the apparent intersections among skillsets. We see data science as a discipline to make sense of data. The techniques and methodologies of data science stem from the fields of computer science and statistics. One of the most well-cited diagrams describing the area comes from Drew Conway where he suggested data science is the intersection of hacking skills, math and stats knowledge, and substantial expertise. This diagram might be a bit of an oversimplification, but it's a great start.

In the obscenity case of Jacobellis v. Ohio (1964), Potter Stewart wrote in his short concurrence that "hard-core pornography" was hard to define, but that "I know it when I see it." This applies to many things including data science. It is hard to define, but you know it when you see it.

So instead of figuring out a good definition, we are going to sketch the history of data science, show you what kind of questions data science can answer, and describe the skills required for being a data scientist. We hope this can give you a better depiction of data science.

If you hit up the Google Trends website which shows search keyword information over time and check the term “data science,” you will find the history of data science goes back a little further than 2004. From the way media describes it, you may feel machine learning algorithms were just invented last month, and there was never “big” data before Google. That is not true. There are new and exciting developments of data science, but many of the techniques we are using are based on decades of work by statisticians, computer scientists, mathematicians and scientists of all types.

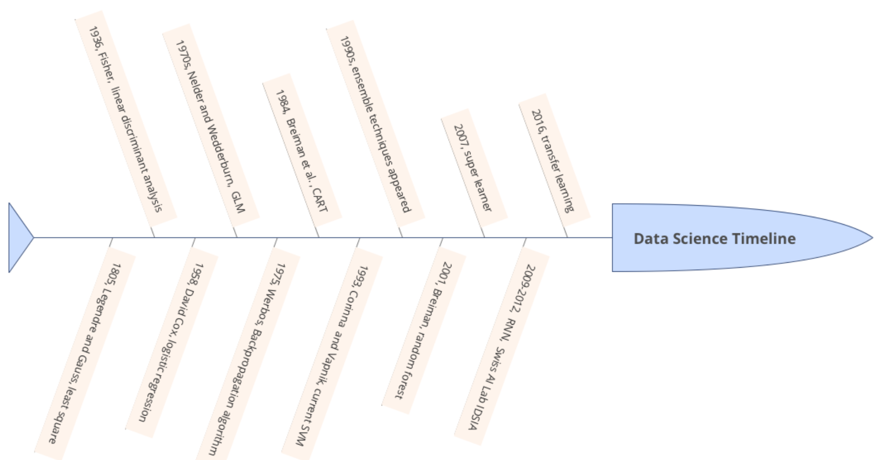

FIGURE 1.1: Data Science Timeline

In the early 19th century when Legendre and Gauss came up the least squares method for linear regression, only physicists would use it to fit linear regression. Now, even non-technical people can fit linear regressions using excel. In 1936 Fisher came up with linear discriminant analysis. In the 1940s, we had another widely used model – logistic regression. In the 1970s, Nelder and Wedderburn formulated “generalized linear model (GLM)” which:

"generalized linear regression by allowing the linear model to be related to the response variable via a link function and by allowing the magnitude of the variance of each measurement to be a function of its predicted value." [from Wikipedia]

By the end of the 1970s, there was a range of analytical models and most of them were linear because computers were not powerful enough to fit non-linear model until the 1980s.

In 1984 Breiman et al. introduced classification and regression tree (CART) which is one of the oldest and most utilized classification and regression techniques. After that Ross Quinlan came up with more tree algorithms such as ID3, C4.5, and C5.0. In the 1990s, ensemble techniques (methods that combine many models' predictions) began to appear. Bagging is a general approach that uses bootstrapping in conjunction with any regression or classification model to construct an ensemble. Based on the ensemble idea, Breiman came up with random forest in 2001. Later, Yoav Freund and Robert Schapire came up with the AdaBoost.M1 algorithm. Benefiting from the increasing availability of digitized information, and the possibility to distribute that via the internet, the toolbox has been expanding fast. The applications include business, health, biology, social science, politics, etc.

John Tukey identified four forces driving data analysis (there was no "data science" then):

1. The formal theories of math and statistics
2. Acceleration of developments in computers and display devices
3. The challenge, in many fields, of more and ever larger bodies of data
4. The emphasis on quantification in an ever wider variety of disciplines

Tukey's 1962 list is surprisingly modern. Let's inspect those points in today's context. There is always a time gap between a theory and its application. We had the theories much earlier than application. Fortunately, for the past 50 years, statisticians have been laying the theoretical groundwork for constructing "data science" today. The development of computers enables us to calculate much faster and deliver results in a friendly and intuitive way. The striking transition to the internet of things generates vast amounts of commercial data. Industries have also sensed the value of exploiting that data. Data science seems certain to be a major preoccupation of commercial life in coming decades. All the four forces John identified exist today and have been driving data science.

1.2 What kind of questions can data science solve?

1.2.1 Prerequisites

Data science is not a panacea, and data scientists are not magicians. There are problems data science can't help. It is best to make a judgment as early in the analytical cycle as possible. Tell your clients honestly and clearly when you figure data analytics can't give the answer they want. What kind of questions can data science solve? What are the requirements for our question?

1. Your question needs to be specific enough

Look at two examples:

- Question 1: How can I increase product sales?
- Question 2: Is the new promotional tool introduced at the beginning of this year boosting the annual sales of P1197 in Iowa and Wisconsin? (P1197 is an impressive corn seed product from DuPont Pioneer)

It is easy to see the difference between the two questions. Question 1 is a grammatically correct question, but it is proper for data analysis to answer. Why? It is too general. What is the response variable here? Product sales? Which product? Is it annual sales or monthly sales? What are the candidate predictors? You nearly can't get any useful information from the questions. In contrast, question 2 is much more specific. From the analysis point of view, the response variable is clearly "annual sales of

P1197 in Iowa and Wisconsin". Even we don't know all the predictors, but the variable of interest is "the new promotional tool introduced early this year." We want to study the impact of the promotion of the sales. You can start from there and move on to figure out other variables need to include in the model by further communication.

As a data scientist, you may start with something general and unspecific like question 1 and eventually get to question 2. Effective communication and in-depth domain knowledge about the business problem are essential to convert a general business question into a solvable analytical problem. Domain knowledge helps data scientist communicate with the language the other people can understand and obtain the required information.

However, defining the question and variables involved don't guarantee that you can answer it. I have encountered a well-defined supply chain problem. My client asked about the stock needed for a product in a particular area. Why can not this question be answered? I did fit a Multivariate Adaptive Regression Spline (MARS) model and thought I found a reasonable solution. But it turned out later that the data they gave me was inaccurate. In some areas, only estimates of past supply figures were available. The lesson lends itself to the next point.

2. You need to have sound and relevant data

One cannot make a silk purse out of a sow's ear. Data scientists need data, sound and relevant data. The supply problem is a case in point. There was relevant data, but not sound. All the later analytics based on that data was a building on sand. Of course, data nearly almost have noise, but it has to be in a certain range. Generally speaking, the accuracy requirement for the independent variables of interest and response variable is higher than others. In question 2, it is data related to the "new promotion" and "sales of P1197".

The data has to be helpful for the question. If you want to predict which product consumers are most likely to buy in the next three months, you need to have historical purchasing data: the last buying time, the amount of invoice, coupons and so on. Information about customers' credit card number, ID number, the email address is not going to help.

Often the quality of the data is more important than the quantity, but the quantity cannot be overlooked. In the premise of guaranteeing quality, usually the more data, the better. If you have a specific and reasonable question, also sound and relevant data, then congratulations, you can start playing data science!

1.2.2 Problem type

Many of the data science books classify the various models from a technical point of view. Such as supervised vs. unsupervised models, linear vs. nonlinear models, parametric models vs. non-parametric models, and so on. Here we will continue on "problem-oriented" track. We first introduce different groups of real problems and then present which models can be used to answer the corresponding category of questions.

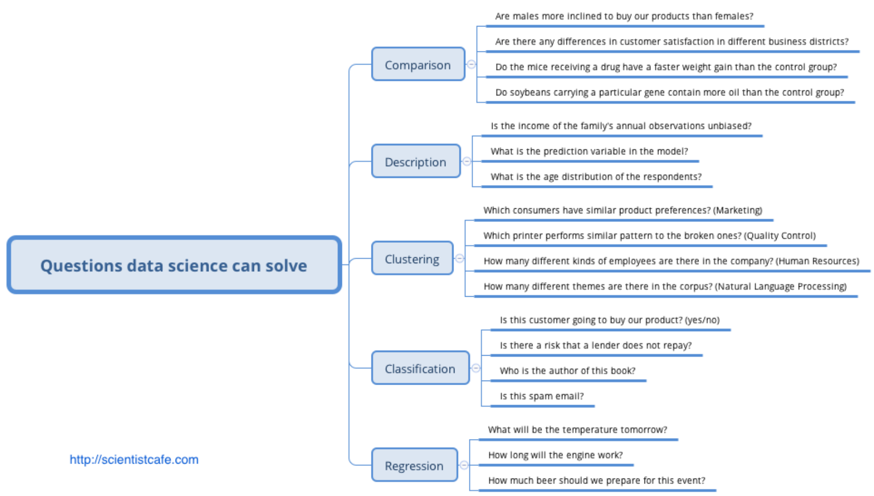

FIGURE 1.2: Data Science Questions

1. Comparison

The first common problem is to compare different groups. Such as: Is A better in some way than B? Or more comparisons: Is there any difference among A, B, C in a certain aspect? Here are some examples:

- Are the purchasing amounts different between consumers receiving coupons and those without coupons?
- Are males more inclined to buy our products than females?
- Are there any differences in customer satisfaction in different business districts?
- Do the mice receiving a drug have a faster weight gain than the control group?
- Do soybeans carrying a particular gene contain more oil than the control group?

For those problems, it is usually to start exploring from the summary statistics and visualization by groups. After a preliminary visualization, you can test the differences between treatment and control group statistically. The commonly used statistical tests are chi-square test, t-test, and ANOVA. There are also methods using Bayesian methods. In biology industry, such as new drug development, crop breeding, mixed effect models are the dominant technique.

2. Description

In the problem such as customer segmentation, after you cluster the sample, the next step is to figure out the profile of each class by comparing the descriptive statistics of the various variables. Questions of this kind are:

- Is the income of the family's annual observations unbiased?
- What is the mean/variance of the monthly sales volume of a product in different regions?
- What is the difference in the magnitude of the variable? (Decide whether the data needs to be standardized)
- What is the prediction variable in the model?
- What is the age distribution of the respondents?

Data description is often used to check data, find the appropriate data preprocessing method, and demonstrate the model results.

3. Clustering

Clustering is a widespread problem, which is usually related to classification. Clustering answers questions like:

- Which consumers have similar product preferences? (Marketing)
- Which printer performs similar pattern to the broken ones? (Quality Control)
- How many different kinds of employees are there in the company? (Human Resources)
- How many different themes are there in the corpus? (Natural Language Processing)

Note that clustering is unsupervised learning. The most common clustering algorithms include K-Means and Hierarchical Clustering.

4. Classification

Usually, a labeled sample set is used as a training set to train the classifier. Then the classifier is used to predict the category of a future sample. Here are some example questions:

- Is this customer going to buy our product? (yes/no)
- Is there a risk that a lender does not repay?
- Who is the author of this book?
- Is this spam email?

There are hundreds of classifiers. In practice, we do not have to try all the models as long as we fit in several of the best models in most cases.

5. Regression

In general, regression deals with the problem of "how much is it?" and return a numerical answer. In some cases, it is necessary to coerce the model results to be 0, or round the result to the nearest integer. It is the most common problem.

- What will be the temperature tomorrow?
- What will be the company's sales in the fourth quarter of this year?
- How long will the engine work?
- How much beer should we prepare for this event?

1.3 Data Scientist Skill Set

We talked about the bewildering definitions of data scientist. What are the required skills for a data scientist?

- Educational Background

Most of the data scientists today have undergraduate or higher degree from one of the following areas: computer science, electronic engineering, mathematics or statistics. According to a 2017 survey, 25% of US data scientists have a Ph.D. degree, 64% have a Master's degree, and 11% are Bachelors.

- Database Skills

Data scientists in the industry need to use SQL to pull data from the database. So it is necessary to be familiar with how data is structured and how to do basic data manipulation using SQL. Many statistics/mathematics students do not have experience with SQL in school. Don't worry. If you are proficient in one programming language, it is easy to pick up SQL. The main purpose of graduate school should be to develop the ability to learn and analytical thinking rather than the technical skills. Even the technical skills are necessary to enter the professional area. Most of the skills needed at work are not taught in school.

- Programming Skills

Programming skills are critical for data scientists. According to a 2017 survey from Burtch Works[1], 97% of the data scientists today using R or Python. We will focus on R in this book, but both are great tools for data science. There is not one "have-to-use" tool. The goal is to solve the problem not which tool to choose. However, a good tool needs to be flexible and scalable.

- Modeling Skills

Data scientists need to know statistical and machine learning models. There is no clear line separating these two. Many statistical models are

[1] http://www.burtchworks.com/2017/06/19/2017-sas-r-python-flash-survey-results/

also machine learning models, vice versa. Generally speaking, a data scientist is familiar with basic statistical tests such as t-test, chi-square test, and analysis of variance. They can explain the difference between Spearman rank correlation and Pearson correlation, be aware of basic sampling schemes, such as Simple Random Sampling, Stratified Random Sampling, and Multi-Stage Sampling. Know commonly used probability distributions such as Normal distribution, Binomial distribution, Poisson distribution, F distribution, T distribution, and Chi-square distribution. Experimental design plays a significant role in the biological study. Understanding the main tenants of Bayesian methods is necessary (at least be able to write the Bayes theorem on the whiteboard and know what does it mean). Know the difference between supervised and unsupervised learning. Understand commonly used cluster algorithms, classifiers, and regression models. Some powerful tools in predictive analytics are tree models (such as random forest and AdaBoost) and penalized model (such as lasso and SVM). Data scientist working on social science (such as consumer awareness surveys), also needs to know the latent variable model, such as exploratory factor analysis, confirmatory factor analysis, structural equation model.

Is the list getting a little scary? It can get even longer. Don't worry if you don't know all of them now. You will learn as you go. Standard mathematics, statistics or computer science training in graduate school can get you started. But you have to learn lots of new skills after school. Learning is happening increasingly outside of formal educational settings and in unsupervised environments. An excellent data scientist must be a lifetime learner. Fortunately, technological advantages provide new tools and opportunities for lifetime learners, MOOC, online data science workshops and various online tutorials. So above all, **self-learning ability** is the most critical skill.

- Soft Skills

In addition to technical knowledge, there are some critical soft skills. These include the ability to translate practical problems into data problems, excellent communication skill, attention to detail, storytelling and so on. We will discuss it in a later chapter in more detail.

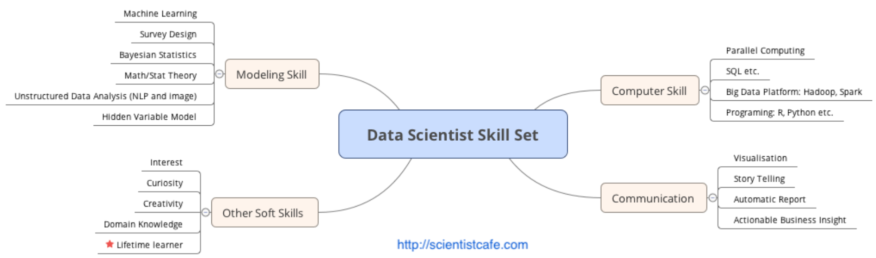

FIGURE 1.3: Data Scientist Skill Set

1.4 Types of Learning

There are three broad groups of styles: supervised learning, reinforcement learning, and unsupervised learning.

In supervised learning, each observation of the predictor measurement(s) corresponds to a response measurement. There are two flavors of supervised learning: regression and classification. In regression, the response is a real number such as the total net sales in 2017, or the yield of corn next year. The goal is to approximate the response measurement as much as possible. In classification, the response is a class label, such as dichotomous response such as yes/no. The response can also have more than two categories, such as four segments of customers. A supervised learning model is a function that maps some input variables with corresponding parameters to a response y. Modeling tuning is to adjust the value of parameters to make the mapping fit the given response. In other words, it is to minimize the discrepancy between given response and the model output. When the response y is a real value, it is intuitive to define discrepancy as the squared difference between model output and given the response. When y is categorical, there are other ways to measure the difference, such as AUC or information gain.

In reinforcement learning, the correct input/output pairs are not present. The model will learn from a sequence of actions and select the action maximizing the expected sum of the future rewards. There is a discount factor that makes future rewards less valuable than current rewards. Reinforcement learning is difficult for the following reasons:

(1) The rewards are not instant. If the action sequence is long, it is hard to know which action was wrong.

(2) The rewards are occasional. Each reward does not supply much information, so its impact of parameter change is limited. Typically, it is not likely to learn a large number of parameters using reinforcement learning. However, it is possible for supervised and unsupervised learning. The number of parameters in reinforcement learning usually range from dozens to maybe 1,000, but not millions.

In unsupervised learning, there is no response variable. For a long time, the machine learning community overlooked unsupervised learning except for one called clustering. Moreover, many researchers thought that clustering was the only form of unsupervised learning. One reason is that it is hard to define the goal of unsupervised learning explicitly. Unsupervised learning can be used to do the following:

(1) Identify a good internal representation or pattern of the input that is useful for subsequent supervised or reinforcement learning, such as finding clusters.

(2) It is a dimension reduction tool that is to provide compact, low dimensional representations of the input, such as factor analysis.

(3) Provide a reduced number of uncorrelated learned features from original variables, such as principal component regression.

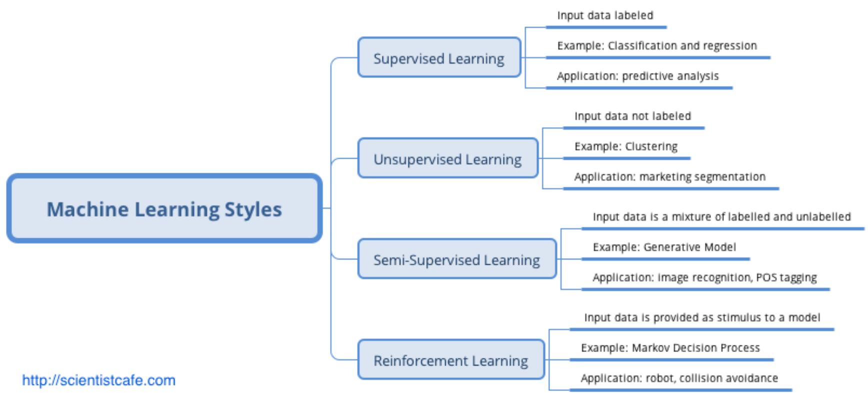

FIGURE 1.4: Machine Learning Styles

1.5 Types of Algorithm

The categorization here is based on the structure (such as tree model, Regularization Methods) or type of question to answer (such as regression).[2] It is far less than perfect but will help to show a bigger map of different algorithms. Some can be legitimately classified into multiple categories, such as support vector machine (SVM) can be a classifier, and can also be used for regression. So you may see other ways of grouping. Also, the following summary does not list all the existing algorithms (there are just too many).

1. Regression

Regression can refer to the algorithm or a particular type of problem. It is supervised learning. Regression is one of the oldest and most widely used statistical models. It is often called the statistical machine learning method. Standard regression models are:

[2]The summary of various algorithms for data science in this section is based on Jason Brownlee's blog "(A Tour of Machine Learning Algorithms)[http://machinelearningmastery.com/a-tour-of-machine-learning-algorithms/]." We added and subtracted some algorithms in each category and gave additional comments.

- Ordinary Least Squares Regression
- Logistic Regression
- Multivariate Adaptive Regression Splines (MARS)
- Locally Estimated Scatterplot Smoothing (LOESS)

The least squares regression and logistic regression are traditional statistical models. Both of them are highly interpretable. MARS is similar to neural networks and partial least squares (PLS) in the respect that they all use surrogate features instead of original predictors.

They differ in how to create the surrogate features. PLS and neural networks use linear combinations of the original predictors as surrogate features [3]. MARS creates two contrasted versions of a predictor by a truncation point. And LOESS is a non-parametric model, usually only used in visualization.

2. Similarity-based Algorithms

This type of model is based on a similarity measure. There are three main steps: (1) compare the new sample with the existing ones; (2) search for the closest sample; (3) and let the response of the nearest sample be used as the prediction.

- K-Nearest Neighbour [KNN]
- Learning Vector Quantization [LVQ]
- Self-Organizing Map [SOM]

The biggest advantage of this type of model is that they are intuitive. K-Nearest Neighbour is generally the most popular algorithm in this set. The other two are less common. The key to similarity-based algorithms is to find an appropriate distance metric for your data.

3. Feature Selection Algorithms

The primary purpose of feature selection is to exclude non-information

[3] To be clear on neural networks, the linear combinations of predictors are put through non-linear activation functions, deeper neural networks have many layers of non-linear transformation

or redundant variables and also reduce dimension. Although it is possible that all the independent variables are significant for explaining the response. But more often, the response is only related to a portion of the predictors. We will expand the feature selection in detail later.

- Filter method
- Wrapper method
- Embedded method

Filter method focuses on the relationship between a single feature and a target variable. It evaluates each feature (or an independent variable) before modeling and selects "important" variables.

Wrapper method removes the variable according to particular law and finds the feature combination that optimizes the model fitting by evaluating a set of feature combinations. In essence, it is a searching algorithm.

Embedding method is part of the machine learning model. Some model has built-in variable selection function such as lasso, and decision tree.

4. Regularization Method

This method itself is not a complete model, but rather an add-on to other models (such as regression models). It appends a penalty function on the criteria used by the original model to estimate the variables (such as likelihood function or the sum of squared error). In this way, it penalizes model complexity and contracts the model parameters. That is why people call them "shrinkage method." This approach is advantageous in practice.

- Ridge Regression
- Least Absolute Shrinkage and Selection Operator (LASSO)
- Elastic Net

5. Decision Tree

Decision trees are no doubt one of the most popular machine learning algorithms. Thanks to all kinds of software, implementation is a no-brainer which requires nearly zero understanding of the mechanism. The followings are some of the common trees:

- Classification and Regression Tree (CART)
- Iterative Dichotomiser 3 (ID3)
- C4.5
- Random Forest
- Gradient Boosting Machines (GBM)

6. Bayesian Models

People usually confuse Bayes theorem with Bayesian models. Bayes theorem is an implication of probability theory which gives Bayesian data analysis its name.

$$Pr(\theta|y) = \frac{Pr(y|\theta)Pr(\theta)}{Pr(y)}$$

The actual Bayesian model is not identical to Bayes theorem. Given a likelihood, parameters to estimate, and a prior for each parameter, a Bayesian model treats the estimates as a purely logical consequence of those assumptions. The resulting estimates are the posterior distribution which is the relative plausibility of different parameter values, conditional on the observations. The Bayesian model here is not strictly in the sense of Bayesian but rather model using Bayes theorem.

- Naïve Bayes
- Averaged One-Dependence Estimators (AODE)
- Bayesian Belief Network (BBN)

7. Kernel Methods

The most common kernel method is the support vector machine (SVM). This type of algorithm maps the input data to a higher order vector space where classification or regression problems are easier to solve.

- Support Vector Machine (SVM)
- Radial Basis Function (RBF)
- Linear Discriminate Analysis (LDA)

8. Clustering Methods

Like regression, when people mention clustering, sometimes they mean a class of problems, sometimes a class of algorithms. The clustering algorithm usually clusters similar samples to categories in a centroidal or hierarchical manner. The two are the most common clustering methods:

- K-Means
- Hierarchical Clustering

9. Association Rule

The basic idea of an association rule is: when events occur together more often than one would expect from their rates of occurrence, such co-occurrence is an interesting pattern. The most used algorithms are:

- Apriori algorithm
- Eclat algorithm

10. Artificial Neural Network

The term neural network has evolved to encompass a repertoire of models and learning methods. There has been lots of hype around the model family making them seem magical and mysterious. A neural network is a two-stage regression or classification model. The basic idea is that it uses linear combinations of the original predictors as surrogate features, and then the new features are put through non-linear activation functions to get hidden units in the 2nd stage. When there are multiple hidden layers, it is called deep learning, another over hyped term. Among varieties of neural network models, the most widely used "vanilla" net is the single hidden layer back-propagation network.

- Perceptron Neural Network
- Back Propagation
- Hopield Network
- Self-Organizing Map (SOM)
- Learning Vector Quantization (LVQ)

11. Deep Learning

The name is a little misleading. As mentioned before, it is multilayer neural network. It is hyped tremendously especially after AlphaGO defeated Li Shishi at the board game Go. We don't have too much experience with the application of deep learning and are not in the right position to talk more about it. Here are some of the common algorithms:

- Restricted Boltzmann Machine (RBN)
- Deep Belief Networks (DBN)
- Convolutional Network
- Stacked Autoencoders
- Long short-term memory (LSTM)

12. Dimensionality Reduction

Its purpose is to construct new features that have significant physical or statistical characteristics, such as capturing as much of the variance as possible.

- Principle Component Analysis (PCA)
- Partial Least Square Regression (PLS)
- Multi-Dimensional Scaling (MDS)
- Exploratory Factor Analysis (EFA)

PCA attempts to find uncorrelated linear combinations of original variables that can explain the variance to the greatest extent possible. EFA also tries to explain as much variance as possible in a lower dimension. MDS maps the observed similarity to a low dimension, such as a two-dimensional plane. Instead of extracting underlying components or latent factors, MDS attempts to find a lower-dimensional map that best preserves all the observed similarities between items. So it needs to define a similarity measure as in clustering methods.

13. Ensemble Methods

Ensemble method made its debut in the 1990s. The idea is to build a prediction model by combining the strengths of a collection of simpler base models. Bagging, originally proposed by Leo Breiman, is one of the earliest ensemble methods. After that, people developed Random Forest (T, 1998; Y and D, 1997) and Boosting method (L, 1984; M and L, 1989). This is a class of powerful and effective algorithms.

- Bootstrapped Aggregation (Bagging)
- Random Forest
- Gradient Boosting Machine (GBM)

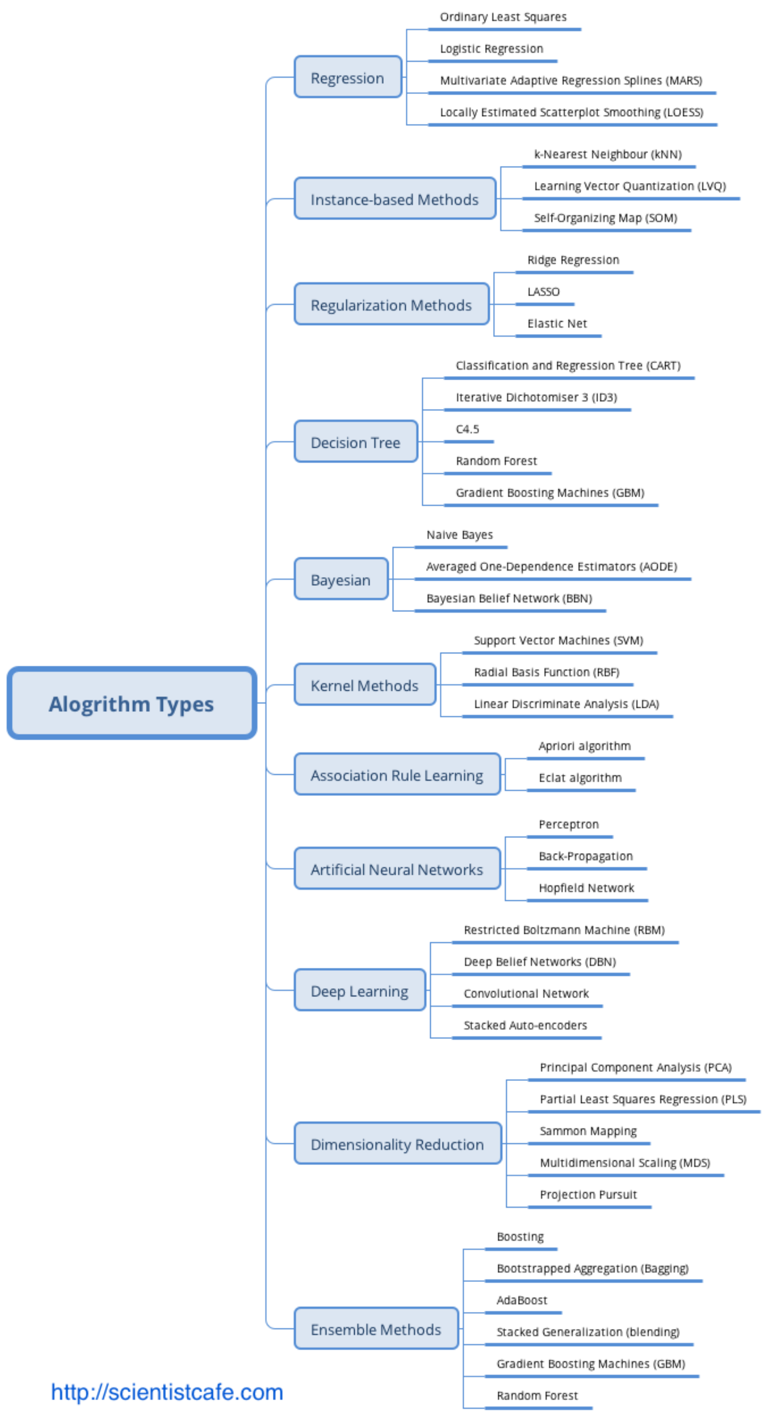

FIGURE 1.5: Machines Learning Algorithms

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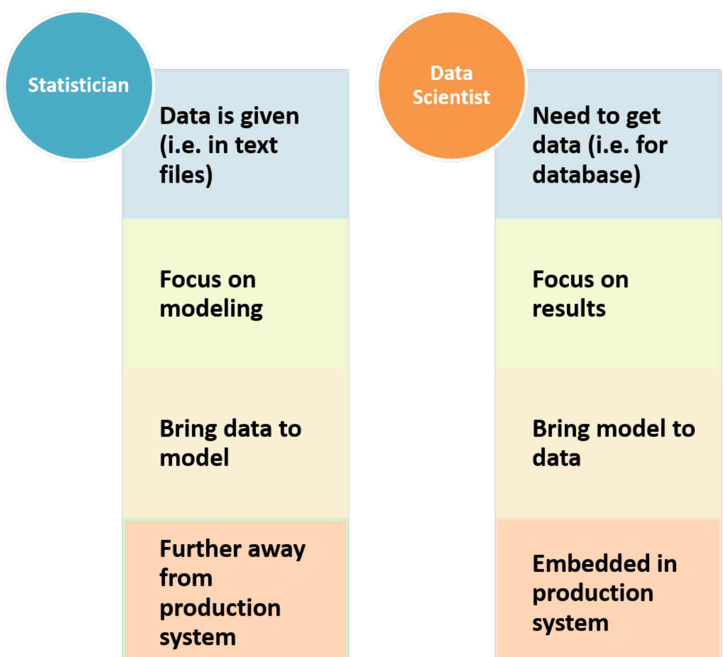
Soft Skills for Data Scientists

2.1 Comparison between Statistician and Data Scientist

Statistics as a scientific area can be traced back to 1749 and statistician as a career has been around for hundreds of years with well-established theory and application. Data Scientist becomes an attractive career for only a few years along with the fact that data size and variety beyond the traditional statistician's toolbox and the fast-growing of computation power. Statistician and data scientist have a lot of common backgrounds, but there are also some significant differences.



Both statistician and data scientist work closely with data. For the traditional statistician, the data is usually well-formatted text files with numbers and labels. The size of the data usually can be fitted in a PC's memory. Comparing to statisticians, data scientists need to deal with more varieties of data: well-formatted data stored in a database system with size much larger than a PC's memory or hard-disk; huge amount of verbatim text, voice, image, and video; real-time streaming data and other types of records. One particular power of statistics is that statistician can fit model and make an inference based on limited data. It is quite common that once the data is given and cleaned, the majority of the work is developed different models around the data. Today, data is relatively abundant, and modeling is just part of the overall effort. The focus is to deliver actionable results. Different from statisticians, data scientists, sometimes need to fit model on the cloud instead of reading data in since the data size is too large. From the entire problem-solving cycle, statisticians are usually not well integrated with the production system where data is obtained in real time; while data scientists are more embedded in the production system and closer to the data generation procedures.

2.2 Where Data Science Team Fits?

During the past decade, a huge amount of data has become available and readily accessible for analysis in many companies across different business sectors. The size, complexity, and speed of increment of data suddenly beyond the traditional scope of statistical analysis or BI reporting as mentioned above. To leverage the big data, many companies have established new data science organizations. Companies have gone through different paths to create their data science and machine learning organizations. There are three major formats of data science teams:

(1) independent of any current organizations and the team report directly to senior leadership;

(2) within each business unit and the team report to business unit

leaders;

(3) within in the traditional IT organizations and the team report to IT leaders.

Companies are different in many aspects, but in general, the most efficient option to mine big data is a team of data scientist independent of business units and IT organizations. The independence enables the data science team to collaborate across business units and IT organizations more efficiently and the independence also provides flexibility and potential to solve corporate level strategic big data problems. For each business units, there are many business unit specific data science related problems and embedding data scientist within each business units is also an efficient way to solve business unit specific data science problems. The full cycle of data science projects from data to decision (i.e. Data -> Information -> Knowledge -> Insight -> Decision) is relatively difficult to achieve if the data science team is part of traditional IT organizations.

2.3 Beyond Data and Analytics

Data scientists usually have a good sense of data and analytics, but data scientist project is more than just data and analytics. A data science project may involve people with many different roles:

- a business owner or leader to identify opportunities in business value; program managers to ensure each data science project fit into the overall technical program development;
- data owners and computation resource and infrastructure owners from IT department;
- dedicated team to make sure the data and model are under model governance and privacy guidelines;
- a team to implement, maintain and refresh the model;
- project managers to coordinate all parties to set periodical tasks so that the project meets the preset milestones and delivery results;

- multiple rounds of discussion of resource allocation (i.e. who will pay for the data science project).

Effective communication and in-depth domain knowledge about the business problem are essential requirements for a successful data scientist. A data scientist will interact with people at various levels ranging from senior leaders who are setting the corporate strategies to front-line employees who are doing the daily work. A data scientist needs to have the capability to view the problem from 10,000 feet above ground, as well as down to the detail to the very bottom. To convert a business question into a data problem, a data scientist needs to communicate using the language the other people can understand and obtain the required information.

2.4 Data Scientist as a Leader

During the entire process of data science project defining, planning, executing and implementation, the data scientist lead needs to be involved in every step to ensure the business problem is defined correctly and the business value and success metric are evaluated reasonably. Corporates are investing heavily in data science and machine learning with a very high expectation of big return. There are too many opportunities to introduce unrealistic goal and business impact for a particular data science project. The leading data scientist need to be the leader in these discussions to define the goal backed by data and analytics. Many data science projects over promise in deliverables and too optimistic on the timeline and these projects eventually fail by not delivering the preset business impact within the timeline. As the data scientist in the team, we need to identify these issues early in the stage and communicate to the entire team to make sure the project has a realistic deliverable and timeline. The data scientist team also need to work closely with data owners to identify relevant internal and external data source and evaluate the quality of the data; as well as working closely with the computation infrastructure team to understand the computation resources (i.e. hardware and software) available for the data science project.

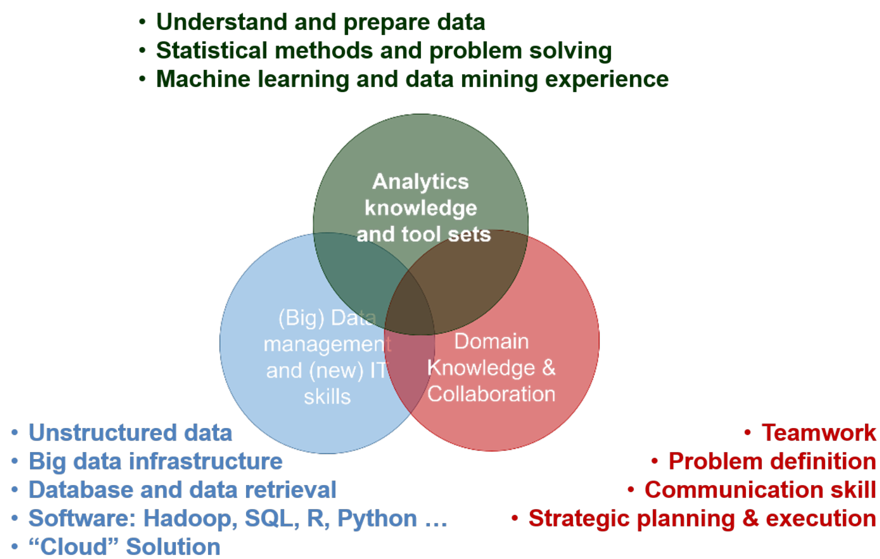
2.5 Three Pillars of Knowledge

The following picture summarizes the needed three pillars of knowledge to be a successful data scientist.

(1) A successful data scientist needs to have a strong technical background in data mining, statistics and machine learning. The in-depth understanding of modeling with the insight about data enable a data scientist to convert a business problem to a data science problem.

(2) A successful data scientist needs some domain knowledge to understand business problem. For any data science project, the data scientist need to collaborate with other team members and effective communication and leadership skills are critical, especially when you are the only data person in the room and you need to decide with uncertainty.

(3) The last pillar is about computation environment and model implementation in big data platform. This used to be the most difficult one for a data scientist with statistics background (i.e. lack computer science or programming skills). The good news is that with the rise of cloud computation big data platform, this barrier is getting easier for a statistician to overcome and we will discuss in more detail in next chapter.



2.6 Common Pitfalls of Data Science Projects

Data science projects are usually complicated, and many of these data science projects eventually fail due to various reasons. We will briefly discuss a few common pitfalls in data science projects and how to avoid them.

- **Solve the wrong problem:** data science project usually starts with a very vague description and a few rounds of detailed discussion with all stakeholders involved are needed to define the busses problem. There will be lots of opportunities to introduce misalignment when mapping the business problem into specific data science methods. Especially when the quality and availability of the data are not as good as what is expected at the first place. If not well-communicated during the project, the final data science solution may not be the right one to solve the business problem. As the data scientist (sometimes the only data scientist) in the room, we must understand the business problem thoroughly and communicate regularly to business partners especially there is a change of status to make sure everyone is aligned with the progress and final deliverables.

- **Over promise on business value:** business leaders usually have high expectation on data science projects and the goal of business value and deliverables sometimes are set unrealistic and eventually beyond the scope of available data and computation resource. As the data scientist (sometimes the only data scientist) in the room, we must have our voice heard based on fact (i.e. data, analytics, and resources) instead of wishful thinking. Backed with fact-based evidence, it is easier to communicate what is a realistic goal for the entire team.

- **Too optimistic about the timeline:** there are lots of uncertainties in data science projects such as the data source availability and data quality, computation hardware and software, resource availability in the business team, implementation team and IT department, as well as project direction change which may delay the final delivery date. To have a better-estimated timeline, get as much detail as possible for all the needed tasks and estimated each task individually and reach out to each team member to confirm their availability. Most importantly, communicate with the entire team if there are blocking factors for the project in a prompt way such that everyone aware of the situation and potential impact on the timeline.

- **Too optimistic about data availability and quality:** the most important asset in data science project is data. Even though we are at the big data age, often there is not enough relevant data for the data science projects. The data quality is also a general problem for data science projects. A thorough data availability and quality check are needed at the beginning of the data science project to estimate the needed effort to obtain data as well as data cleaning.

- **Model cannot be scaled:** be careful if you use a subset of data to fit the model and then scale it to the entire dataset. When developing the model using a smaller dataset, we must keep in mind how much computation resources needed for the whole dataset. With limited computation resource, it is important to maximize the computation time in production to a reasonable level based on the business application when fits the model with a sample dataset.

- **Take too long to fail:** data science projects usually are trying to push the boundary of current applications to new territory, people do not expect all data science projects to be successful. Fail fast is good practice such that we can quickly find a better way to solve the problem. A data scientist needs to have an open mindset to not stuck with one idea or one approach for a long time to avoid taking too long to fail.

3

References

Bibliography

Donoho, D. (2015). 50 years of data science.

L, V. (1984). A theory of the learnable. *Communications of the ACM*, 27:1134–1142.

M, K. and L, V. (1989). Cryptographic limitations on learning boolean formulae and finite automata. In *In "Proceedings of the Twenty-First Annual ACM Symposium on Theory of Computing*.

T, H. (1998). The random subspace method for constructing decision forests. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 13:340–354.

Y, A. and D, G. (1997). Shape quantization and recognition with randomized trees. *Neural Computation*, 9:1545–1588.