Data Science and Ebola

Inaugural Lecture by

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Addressing the Audience

Mevrouw de Rector-Magnificus,
Mijnheer de Decaan en Leden van het bestuur van de Faculteit Wiskunde en
Natuurwetenschappen,
Dames en heren hoogleraren,
Dames en heren van de wetenschappelijke en de ondersteunende staf,
Dames en heren studenten,
En voorts Gij allen die deze plechtigheid met uw aanwezigheid vereert,

Deze aanspreektitel vormt de brug tussen het verleden en het heden.
De tekst wordt in het Engels uitgesproken.

On 4 September 2014, shortly after the start of the academic year, the Leiden Centre of Data Science (LCDS) was officially opened, in this same historic building. On that day the university recognized the importance of this new field of science. The opening speeches were by Trevor Hastie, professor of Mathematical Sciences at Stanford University, and by Prince Constantijn van Oranje, who told us about his work for the Digital Agenda of the European Commission. Many people have since then stressed the importance of data. By the end of 2014 both the European Commission and the Netherlands government named data a key asset for the economy. Both established a data strategy, and both announced substantial funding for data science research. Data may well have been the second most used word of last year.

Today, everybody and everything produces data. People produce large amounts of data in social networks and in commercial transactions. Medical, corporate, and government databases continue to grow. Ten years ago there were a billion Internet users. Now there are more than three billion, most

of whom are mobile.[1] Sensors continue to get cheaper and are increasingly connected, creating an *Internet of Things*. The next three billion users of the Internet will not all be human, and will generate a large amount of data.

In every discipline, large, diverse, and rich data sets are emerging, from astrophysics, to the life sciences, to medicine, to the behavioral sciences, to finance and commerce, to the humanities and to the arts. In every discipline people want to organize, analyze, optimize and understand their data to answer questions and to deepen insights.

The availability of so much data and the ability to interpret it are changing the way the world operates. The number of sciences using this approach is increasing. The science that is transforming this ocean of data into a sea of knowledge is called *data science*. In many sciences the impact on the research methodology is profound—some even call it a paradigm shift.

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[1]source: http://internetlivestat.com

Chapter 2

Ebola as Data Challenge

First I will address the question of why there is so much interest in data. I will answer this question by discussing one of the most visible recent challenges to public health of the moment, the 2014 Ebola outbreak in West Africa.

2.1 United Nations Global Pulse

Aid organizations recognize the necessity of correct information for effective humanitarian aid, especially when disasters have disrupted the functioning of government institutions. The United Nations has started Global Pulse, a flagship data science initiative of Secretary-General Ban Ki-moon. The goal of Global Pulse is to accelerate discovery, development and adoption of data science innovations for sustainable development and humanitarian action.[1] Global Pulse was started in 2014.

The United Nations issued a report to the Secretary-General entitled *A World That Counts: Mobilising the Data Revolution for Sustainable Development*. At the presentation of the report, the co-chair of the Expert Group, Enrico Giovannini, noted that: "We live in a world that faces rapidly-evolving humanitarian and development challenges, as the Ebola epidemic so tragically proves. Governments, companies, NGOs and individuals need good data to know where problems are, how to fix them, and if the solutions are working. But current data are not good enough. Too many people and issues are not counted or measured, there are huge and growing inequalities between the information-rich and the information-poor."

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[1]http://unglobalpulse.org

2.1.1 The 2014 Ebola Outbreak

Outbreaks of contagious diseases lead to severe disruptions of society, not to mention the loss of life in all its tragedy. The history of the fight against diseases shows some successes, such as against the plague and pox, but there are still many diseases that we have not been able to eradicate, such as malaria, tuberculosis, and influenza.

Ebola is one such unsolved disease. The first reported outbreak of Ebola was in 1976, in the rural village of Yambuku in Zaire, 100 km from the *white water river*, or *Ebola*, as it is called in the local tongue. The disease was so terrible, that, to avoid stigma to the villagers of Yambuku, it was named after the far away river instead (cf., Wordsworth (2014)). Small outbreaks of Ebola have been occurring regularly in the past. They have been reported in Zaire and Sudan, in 1995, in 2000, in 2003, in 2007, and in 2012. The most recent outbreak is the 2014 outbreak, in West Africa. This was the first outbreak in an urban environment. The outbreak started in Guinea, and spread to Liberia and Sierra Leone.

Researchers traced the outbreak to a two-year old child who died in December 2013. In this outbreak, half of the people who suffered from the disease died. As this outbreak occurred in an urban environment, it spread much quicker than previous outbreaks, and caused more fatalities. By early 2015 this number had reached 10,000. As the outbreak progressed, many hospitals, short on staff and supplies, became overwhelmed and closed, leading health experts to state that this may be causing a death toll that is likely to exceed that of the disease itself. Hospital workers are especially vulnerable to catching the disease since they can easily come into contact with highly contagious body fluids. The World Health Organization (WHO) reported that ten percent of the dead have been healthcare workers.

The virus is thought to reside in fruit bats. As of this writing, there are no approved vaccines or adequate treatments for Ebola, although trials are under way. The disease spreads between humans by contact with bodily fluids, such as blood, or sweat. The incubation period is long, between one and three weeks. This long incubation period is one of the factors that allow the disease to spread so effectively. Furthermore, Ebola symptoms initially resemble the flu or malaria. The outbreak happened in countries with a poor health infrastructure (Van de Walle & Comes, 2014). Infected people are often misdiagnosed, are not treated, and thus unknowingly infect healthy people.

Past outbreaks were brought under control within a few weeks; the 2014 Ebola outbreak is the first one to reach epidemic proportions. The epidemic has a significant economic effect. People are fleeing from affected areas, cre-

ating a refugee problem and weakening the economy. Movement of people away from affected areas has disturbed agricultural activities. The UN Food and Agriculture Organisation (FAO) warned that the outbreak endangered harvest and food security in West Africa. Liberia and Sierra Leone struggled and initially failed to contain the disease. On 8 August 2014, the World Health Organization declared the outbreak an international emergency.

The lack of reliable data is a serious contributing factor to the 2014 Ebola outbreak, according to the World Health Organization. Humanitarian aid agencies cannot respond appropriately; misinformation leads to widespread fear among the population.

2.1.2   Three Data Challenges

To address the lack of data, innovative data analysis methods can be a help. They can improve the reliability of data, and support reducing the effects of tragedies, as the United Nations report on the Global Pulse indicates. In this way, data science is changing the way that humanitarian problems are solved in our world.

As this lecture is being prepared in early 2015, aid workers and scientists have worked hard to contain the effects of the Ebola outbreak. There are three main challenges for data scientists who are attempting to resolve the tragedy. These are: (1) diagnosis, (2) epidemiological spread, and (3) treatment and drug discovery. I will now discuss these challenges.

2.2   Diagnosis

The first challenge is in diagnosing Ebola. Conventional diagnostic tests require specialised equipment and highly trained personnel. There are few suitable testing centers in West Africa, which leads to delays in diagnoses. In December 2014, a WHO conference in Geneva aimed to work out which diagnostic tools could be used to identify Ebola reliably and more quickly. The meeting sought to identify tests that can be used by untrained staff, do not require electricity or can run on batteries or solar power and use reagents that can withstand temperatures of 40°C. On December 29, 2014, the US Food and Drug Administration approved a test on patients with symptoms of Ebola.

2.2.1   Reliable Health Data

The difficulty in diagnosing Ebola is one of the reasons for the disease to spread unnoticed. Doctors and hospitals are underequipped and therefore underre-

port Ebola cases. Months passed between the first Ebola case and its reporting. Data scientists have worked to address the unreliability of Ebola data. The Northeastern University has published an online model which assesses the progression of the epidemic based on simulations of a typical epidemic spread. The analysis is presented as a live paper that is continuously updated with new data, projections and analysis (Gomes et al., 2014).

To acquire more reliable data, efforts have moved to crowdsourcing initiatives that use mobile phones and SMS service. Since the SMS and voice data are location-specific, it is possible to create maps that correlate public sentiment to location. Others have created cheap alternative diagnostic tools, such as checklist apps for smartphones. The apps may reduce fear and uncertainty among the population, possibly reducing the refugee problem and its disruptive effect on the fragile economies (cf., Parejo & Maestre (2015)).[2]

2.2.2 Open Data, Open Government

Knowledge is power, and governments and organizations are often protective of their data (see, e.g., Van de Walle & Comes (2014)). However, as the scale of the outbreak became clear, governments and organizations started to cooperate in exchanging data on the disease. Many organizations eventually joined open data initiatives that allowed scientists access to their data, to be combined with other open data sources.

In the midst of the fast-moving crisis, traditional methods for solving problems did not move fast enough. Volunteer efforts have sprung up in Africa and around the world in a combination of open data, analytics software, and crowdsourcing. IBM has set up an African Open Data Initiative to help African countries tap open data as a means of addressing health, infrastructure and economic challenges. The World Health Organization provided data. In New York a grassroots Ebola Open Data Jam was organized.[3] The UN Office for the Coordination of Humanitarian Affairs set up a Humanitarian Data Exchange.[4] The government of Sierra Leone created its own Open Data initiative.[5] The Ebola epidemic caused the Liberia Government to provide data on their government to the outside. In this way it faciltated the step towards Open Government.[6]

These open data initiatives are of great value since they allow different scientists to work on the data, to combine data sources, and to improve their

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[2]http://www.appsagainstebola.org/

[3]http://eboladata.org

[4]https://data.hdx.rwlabs.org

[5]http://www.ogi.gov.sl

[6]http://www.opengovpartnership.org/country/liberia

models. For example, one of the findings of the project for the Global Data on Events, Location and Tone (GDELT) is that a global monitoring of internet and media news can provide a picture of the unfolding of the outbreak that is as accurate as ground truth data,[7] only much faster.[8]

The availability of different data sources allows data to be triangulated, or cross-checked, which improves data quality. Models have been made to visualize the spread of the disease using heat maps that correlate locations to public sentiment, migration, infections, and fatalities. Special tools, such as the Spatiotemporal Epidemiological Modeler tool, are designed to help scientists and public health officials create real time models of emerging infectious diseases.[9]

2.3   Epidemiological Spread

The second challenge is how to model reliably the spread of the epidemic. Epidemiologists traditionally have to rely on anecdotal information, on-the-ground surveys, and police and hospital reports. This type of data is often collected too slowly to curb the spread of the disease. Scientists have been working under time pressure to develop novel methods to map the spread more quickly and more precisely. Below I discuss two methods, viz. analyzing mobile phone data (subsection 2.3.1) and improving contact tracing (subsection 2.3.2).

2.3.1   Mobile Phone Data

The first method is to analyze mobile phone data. Mobile phones are nowadays widely owned in even the poorest countries in Africa. They are a rich source of data in a region where only a few other reliable sources are available. Orange Telecom in Senegal handed over anonymized voice and text data from 150,000 mobile phones to a Swedish non-profit organization, whose data analysts drew up detailed maps of typical population movements in the region. Authorities and aid workers could then see where the best places were to set up treatment centers. Authorities also used this information to find the most effective ways to restrict travel in an attempt to contain the disease.

A second way in which phone data is used, is by tracking the number of calls to helplines. A sharp increase from one particular area could suggest an outbreak and alert authorities to direct more resources to that area. Software

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[7]https://keystoneaccountability.wordpress.com/tag/nick-van-praag/

[8]http://gdeltproject.org,

[9]https://www.eclipse.org/stem/

companies are helping to visualize this data and overlay other existing sources of data from ground truth data to build up a richer picture.

Mobile phone data can be used to improve the accuracy of epidemiological models. Epidemiology uses advanced statistics to model the spread of a disease, often based on historical data, the level of contagiousness of the disease, and on behavioral factors. Dynamic models combine historical data with current field measurements. The dynamic models can be more precise in their prediction of the spread of a disease than static historical models. The difference in accuracy can be large, with serious consequences for policy makers.

As a case in point, we mention a report of September 2014 by the Center of Disease Control. It analyzes the impact of underreporting and suggests correction of case numbers by a factor of up to 2.5. With this correction factor, approximately 21,000 total cases were estimated for the end of September 2014 in Liberia and Sierra Leone alone. The same report predicts that the number of cases could reach 1.4 million in Liberia and Sierra Leone by the end of January. Two months later, at a congressional hearing, the director of the CDC said that the number of Ebola cases was no longer expected to exceed 1 million, moving away from the worst-case scenario that had been previously predicted.

New data allow new mathematical models to be validated. One model that has attracted attention is the IDEA model, a straightforward two parameter mathematical model that appears to model the spread of the disease well (cf., Fisman et al. (2014)).

Access to real time data, such as the measurement of migration patterns through mobile phone tracking, is of great value to improve epidemiological models. Incorporating data from different sources into simulation models allows data triangulation to predict the spread of the disease better. Improving the accuracy of statistical models is important not only for better targeting of relief work, but also for improving the reputation of aid organizations as providers of trustworthy information.

2.3.2   Contact Tracing

The second method for better mapping the spread of the disease is to improve contact tracing. Contact tracing is an important method (1) for understanding the spread of Ebola and (2) for acquiring correct numbers on the size of the epidemic. Contact tracing requires effective community surveillance so that a possible case of Ebola can be registered and diagnosed. Subsequently everyone who has had close contact with the patient must be found and tracked for 21 days. This requires careful record keeping and many properly trained and equipped staff. There is a substantial effort to train volunteers and health work-

ers, sponsored by USAID. According to WHO reports, 25,926 contacts from Guinea, 35,183 from Liberia and 104,454 from Sierra Leone were listed and being traced at the end of 2014.

Contact tracing is labor intensive. Patients are interviewed and their relatives over the past period are contacted to establish how they were likely infected, and whom they could have likely infected. Contacts are watched for 21 days, to see whether they develop symptoms of the illness. Thus, a social graph of the patient is built. By combining social graphs of people in an area an overall view of the network of the disease in a certain area and time period can be created.[10]

Estimating the spread of the disease is difficult. A study published in December 2014 by Scarpino et al. (2014) found that transmission of the Ebola virus occurs principally within families, in hospitals and at funerals. The data, gathered during three weeks of contact tracing showed that the third person in any transmission chain often knew both the first and second person. The authors estimated that between 17 percent and 70 percent of the cases in West Africa are unreported. Prior projections had estimated a much higher figure. The study concludes that the epidemic is not as difficult to control as feared, if rapid, vigorous contact tracing and quarantines are employed.

Traditional contact tracing methods involve traveling to patients and interviewing them. Online social networks and contact lists of patients provide quick information about the kind of network and travel patterns of patients. Patients with many contacts and an active travel pattern can be quickly identified, allowing more efficient use of scarce tracing personnel. Current manuals do not prescribe taking online information into account. Apps are being developed to ease the process of contact tracing.[11] We conclude that innovative contact tracing methods such as analyzing online social networks, mobile phone data and apps can speedup the process of contact tracing, to better map the epidemiological spread.

2.4 Treatment & Drug Discovery

The third challenge that I will discuss is related to the prevention of Ebola. It concerns treatment and drug discovery. Pharmacologists have developed a range of high performance drug discovery techniques over the past years. They are used intensively to find a cure for Ebola.

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[10]CDC Methods for Implementing and Managing Contact Tracing for Ebola Virus Disease in Less-Affected Countries, Centers for Control & Prevention, 2014

[11]http://www.appsagainstebola.org

2.4.1 Treatment

At the time these words were written there is no approved vaccine for Ebola, despite a large effort by the pharmaceutical industry. In addition, there is no cure or specific treatment that is currently approved. Treatment is primarily supportive in nature, as survival chances are improved by early care with rehydration and symptomatic treatment. A number of experimental treatments are being considered for use in the context of this outbreak, and are currently in clinical trials. Patient data is recorded to understand the most effective combination of therapies. In other diseases a well balanced combination of symptomatic treatment has been shown to increase both life expectancy and the quality of life of patients. Transparent access to reliable patient records for doctors and scientists is necessary for effective treatment development.

2.4.2 Drug Discovery

Finding a preventive vaccine for Ebola is of prime importance. According to a recent study by the US National Institute of Allergy and Infectious Diseases the scientific community is still in the early stages of understanding how infection with the Ebola virus can be treated and prevented. Many Ebola vaccine candidates have been developed in the decade prior to 2014, but none has yet been approved for clinical use in humans. Several promising vaccine candidates protect nonhuman primates (usually macaques) against lethal infection, and some are now going through the clinical trial process.

The process of drug discovery has advanced to a state where many steps have been automated. High throughput screening is a method for scientific experimentation in drug discovery. It uses robotics, data processing and control software, and includes sensitive detectors and devices for handling liquids. High throughput screening allows a researcher to conduct quickly millions of chemical, genetic, or pharmacological tests. Researchers have developed computational methods to analyze these test results.

Results from high throughput screening are used to refine simulation models of the virus, in order to design a vaccine. Simulation data can then be checked with in-vitro observations.

Pharmacology and molecular biology are active fields of research, where many results on gene-disease findings and related drugs are published. In addition to analyzing *databases* of molecules and proteines the *publications* themselves allow a drug discovery method based on text mining and statistics. In this method textual correlations in scientific papers are analyzed. A high textual correlation indicates an increased possibility of a relation between molecules

and diseases, warranting further research. The advantage of such in-silico drug discovery are (1) the low cost and (2) the systematic nature of the search, allowing a much wider investigation of acceptable relations than is possible with traditional methods.

2.5   Ebola: Three Challenges for Data Science

At this point, we have discussed three challenges where data science is helping to resolve the Ebola tragedy. The outbreak occurred in countries with a poor health infrastructure, and a lack of reliable data. Governments and organizations learned the importance of opening up their data. Data scientists could then work on (1) better methods for diagnosis, (2) new online epidemiological models, and (3) developing vaccines and treatment methods.

Ad (1) Open data initiatives improve the quality of data about the outbreak. Novel methods such as smartphone self assessment apps have been developed, and the movement of people is analyzed based on data from mobile phones.

Ad (2) New online epidemiological models are developed that help simulate the spread of the disease based on data that is continuously being updated. A relatively new area is the analysis of online social networks and call information for contact tracing, to improve the accuracy and efficiency of manual methods.

Ad (3) Pharmacologists are working hard to develop vaccines and treatment drugs for Ebola, making use of high throughput drug discovery methods and data analysis in trials.

In conclusion, data science has permeated the methods of doctors, aid workers, epidemiologists, and pharmacologists, helping them to fight the disease.

Let us now look into more detail at the technologies that data science is using. It allows us to understand future developments for Ebola, and for other domains.

Chapter 3

Data Science Technologies

In the past, data collection and processing techniques were limited in their power and versatility. In the last decade techniques have progressed considerably. For Ebola a wide range of data sources are used, such as mobile phone data, diagnostic app data, social network data, and advanced mathematical models. Combining these kinds of data requires new data processing technologies.

We will now describe three techniques in more detail. (1) For *diagnosis* we will look at data quality and representation techniques, (2) for *epidemiological spread* we will look at analysis techniques for diverse and large data sets, and (3) for *treatment* we will look at high performance data analysis techniques.

3.1 Data Quality & Representation

I will start with techniques for data quality and representation that are used in the diagnosis part of the Ebola outbreak.

3.1.1 Quality of Ebola Data

An important aspect of data science is data quality. In many projects the most time consuming task is ensuring the quality of the data: cleaning the data, and checking for missing and inconsistent values (see, e.g., Rahm & Do (2000)). For Ebola, gathering high quality data is a difficult challenge, and alternative sources were sought, such as mobile phone data and internet news postings. These additional sources allow data to be triangulated so that the quality increases. Also, data can be collected more quickly and is broader in scope.

3.1.2   Knowledge Representation Techniques for Ebola

In diagnosing Ebola data from different sources is collected in different data sets. It is in combining data from different areas where the real power of data science lies: triangulating data to improve data quality, and also, finding unexpected patterns. To be able to compare items from different data sets, the data must be represented in an organized and comparable manner. The field of knowledge representation studies this aspect. It uses techniques such as semantic networks and automated inferencing to organize knowledge in taxonomies and ontologies. Semantic web techniques for linked open data allow automatic inference of diverse kinds of data, such as social network data (cf., Groth et al. (2012)). Social and semantic network techniques are areas of active research. Their use in helping to diagnose Ebola cases illustrates how fundamental research and real world challenges can go together.

3.2   Analysis Techniques for Diverse & Large Data Sets

I will now discuss two techniques for analysis of diverse and large data sets that are used in modeling the epidemiological spread of the Ebola outbreak.

3.2.1   Diverse Data Sets

Epidemiology makes good use of statistics and data analysis techniques. Developers of statistical methods have a history of standardizing their best algorithms into libraries and software packages. Well known packages that are used in epidemiology are SPSS (Meulman & Heiser, 2001; Field, 2009), Weka (Witten et al., 2011), and R (R Core Team et al., 2012). These packages have paved the way for the use of data analysis techniques in epidemiology and in other sciences.

   The data sources that are used for tracking the spread of the 2014 Ebola outbreak are diverse and go beyond traditional tables of numerical data. Data can be text documents, sound, pictures, even video, and data from motion sensors. Data can be dynamic, for example an incoming stream of messages or video. Conventional, linear, statistical methods are not suited to analyze the data from the Ebola outbreak. Efforts to analyze this kind of high dimensional data have yielded new statistical and machine learning techniques (see, e.g., Hastie et al. (2009); Johnstone & Titterington (2009); Takes (2014); Schraagen (2014)). As the Ebola case shows, still more techniques are needed, and the advanced techniques must be packaged in a way that is accessible for epidemiologists and other scientists.

3.2.2   Large Data Sets

Current data sets are larger than before, have a more diverse structure than before, and change more frequently than before. Finding answers in such large, unstructured, data sets requires intelligent search algorithms that adapt to the search space at hand. Many years ago, in Rotterdam and Edmonton, I started to work in this field, as part of my PhD research.

For analyzing large data sets a variety of adaptive search techniques exists, ranging from stochastic methods (see, e.g., Hoos & Stützle (2004); Ruijl et al. (2014a,b)), multiple-objective optimization (see, e.g., Koch et al. (2015)), evolutionary algorithms (see, e.g., Bäck et al. (2013); Bäck (2014)), to new versions of neural networks (see, e.g., Krizhevsky et al. (2012)). These techniques have shown remarkable success, although many challenges remain. In subsection 5.2.2 I will describe ideas for future research.

3.3   High Performance Drug Discovery Techniques

In searching for vaccines, high performance data analysis techniques are heavily used. I will briefly discuss techniques from high performance computing, a field in which I worked as a postdoc, first in Cambridge at MIT, and later in Amsterdam at the VU.

Quickly analyzing large data sets requires fast algorithms and fast computers. Initially supercomputers were used for numerical modeling, for applications such as computational fluid dynamics, for weather prediction, and for simulations ranging from nuclear to galactic processes.

In contrast, many of the drug discovery techniques for Ebola involve classification and discrete choice (both for epidemiology and for vaccine discovery). These problems require the application of combinatorial methods, as used, for example, in route planning problems, scheduling (see, e.g., Plaat (1996); Hoos & Stützle (2004)), or for searching for relations between genes and diseases in large databases. Together, methods from numerical and combinatorial analysis comprise data science. There have been great advances in high performance computing, combinatorial optimization, and databases (see, e.g., Plaat et al. (2001); Boncz et al. (2008); Dean & Ghemawat (2008); Seinstra et al. (2011); Engle et al. (2012); Mirsoleimani et al. (2014)). These have enabled the application of supercomputing to fields as diverse as the life sciences, the social sciences, and the humanities.

Due to the increased need for data analysis the worldwide demand for compute power is increasing sharply. In this respect it is remarkable to see that the

Netherlands investment in scientific compute power is not keeping pace. Our place in the worldwide list of supercomputers, the TOP 500, is embarrassingly low, and certainly not commensurate with that of a data economy.[1]

3.4   Data Science: Three Techniques for Ebola

We have discussed three techniques that are used to resolve the Ebola tragedy. These are techniques for (1) collecting high quality data and organizing the data so that combinations between data sets of a diverse structure can be made, (2) for the analysis of large and diverse data sets, using adaptive techniques for high dimensional data sets, and (3) high performance drug discovery techniques. High performance techniques are necessary since the size of the data, especially when combinations are made, quickly becomes too large for ordinary computers.

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[1]http://top500.org

Chapter 4

Multidisciplinary Cooperation

We have now surveyed data science techniques that are used for Ebola and that have changed the way in which the disease is handled. For a moment we will digress and look at other applications, outside the life sciences, in which data science is causing a similar change. We will start with astronomy.

4.1 Astronomy

In astronomy, the Low Frequency Array (LOFAR) radio telescope consists of 25,000 small antennas that are spread out over a larger area to effectively form one large virtual antenna (Röttgering et al., 2006; Haarlem et al., 2013). LO-FAR's antennas together generate so much raw data that it has to be reduced before it can be stored for further processing and analysis (cf., De Vos et al. (2009)). A dedicated supercomputer, BlueGene/L, has been built to do the signal processing of LOFAR (Romein et al., 2006, 2011). LOFAR's design has not only been made possible by advanced sensor technology, but also by fast signal processing algorithms and large compute power.

4.2 Physics

In physics, particle experiments generate large amounts of data. On the 4th of July of 2012 one of the most important scientific discoveries in physics was announced: two independent experiments reported results that were consistent with the detection of the Higgs boson (Aad et al., 2012; Chatrchyan et al., 2012), the last elusive particle from the standard model. A year later Peter

Higgs was awarded the Nobel prize, together with Francois Englert.[1] Calculations from almost 50 years ago, predicting the particle's existence, had been proven correct.

It has been reported that around 100 Petabyte of data has been generated in the Large Hadron Collider at CERN in these experiments. To put that amount in perspective, my somewhat older laptop has a storage capacity of 128 Gigabyte. The amount of data stored at CERN would require 800,000 of those laptops to store it.

In addition to experimentalists, theorists too work with large amounts of data. Ever since the 1960s theoretical physicists have been using computers to manipulate large formulas to predict experimental results. Veltman and 't Hooft used a special computer algebra system for the calculation for which they received their Nobel prize in 1999. Inspired by their system Jos Vermaseren developed an improved system called FORM, to work with such large formulas (Vermaseren, 2000; Ueda & Vermaseren, 2014).[2]

For the next generation of particle experiments even more complex calculations are required. In the HEPGAME project, for which we gratefully acknowledge EU funding through the ERC Advanced scheme, Jos Vermaseren, Jaap van den Herik and I work, with our PhD students and postdocs, on advanced combinatorics and physics to make these complex calculations in FORM possible (Vermaseren et al., 2013; Ruijl et al., 2014b; Mirsoleimani et al., 2014).[3]

4.3 Law Enforcement

One field with a natural interest in the behavior of their "customers" is law enforcement. Activities to reduce terrorism, crime, hooliganism, and jihadism are becoming increasingly driven by information.

Data-driven methods are credited with modern policing successes in Los Angeles, New York, and other cities.[4] Our national police is also gathering data to increase effectiveness, by correlating crime figures with police actions. *Intelligent* blue, instead of more blue, is the new motto. Many police forces are experimenting with intelligence led policing (Meesters, 2014). Other data-driven methods have also shown success. Combining scenario methods with data analytics can be used to anticipate criminal behavior to some degree (De Kock,

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[1]http://press.web.cern.ch/press-releases/2011/12/atlas-and-cms-experiments-present-higgs-search-status

[2]http://www.nikhef.nl/~form

[3]http://hepgame.org

[4]http://www.governing.com/topics/public-justice-safety/Data-driven-Policing.html

2014).

4.4   Commerce

Data science is an important factor in the online and offline economy. In book-selling (Amazon) and online video (YouTube, Netflix) the volume of buying decisions and views allows statistically significant personalized recommendations to be computed. These recommendations drive much of sales. Data warehouses have become core systems, for example, for calculating online ticket prices in the hospitality and travel industry.

4.5   Regulation

Increasingly we live our lives online, where expectations about privacy may not hold. Technology is proving a difficult topic for regulators that wish to protect our rights. As in all of our society, moral and ethical issues arise, and research into the philosophical and legal aspects of behavioral data collection is an important area (see, e.g., Van den Berg & Leenes (2013); Van den Berg & van der Hof (2012); Van Den Herik et al. (2014)). Active legal research is needed, and legal scholars need to have an adequate technological understanding (Prins, 2014; Van den Berg & Keymolen, 2013; Van der Zwaan et al., 2014).

Chapter 5

Outlook

Having looked at how data science is used for Ebola and other applications, it is now time to look into the future. First we will discuss how data science improves the chances of preventing future virus outbreaks. Next we will discuss plans for data science research. Finally, we will look at data science in Leiden.

5.1   Future Ebola Outbreaks

The medical history of conquering diseases is one of many successes, although important challenges remain.

The loss of some 10,000 lives since the 2014 Ebola outbreak and the ensuing human and social disruption are deeply tragic. So tragic, and so large is the impact of the outbreak, that it caused scientists, volunteer efforts, and the international community (1) to work around the clock to improve diagnosis techniques for the disease, (2) to improve the tracking of the spread of the disease, (3) to gather information on patient treatment, and (4) to work on experimental vaccines.

Due to the urgency of the situation governments and organizations opened up their data, and researchers used the latest data science techniques in their approaches. Regardless of the reason novel medical and data science methods were created. The accuracy of epidemiological models improved greatly—causing predictions to be adjusted by more than an order of magnitude (see section 2.3.1). Pharmacologists have been working hard to create vaccines. At the time of this writing the first vaccines have been scheduled for phase 3 trials at the end of 2015.

Unless vaccines will become available at a low cost and at a wide scale, it is likely that Ebola incidents will continue to occur. However, with open gov-

ernments and the concerted effort from the international scientific community, new diagnostic tools, epidemiological models, and treatment and drug discovery methods have been developed. Together these will likely prevent outbreaks of the scale of 2014. Many of the lessons, such as advances in dynamic epidemiological modeling, are likely to help in containing other diseases as well.

The availability of open data and data science technology are causing fundamental changes in our science and in our society, as the Ebola case illustrates. Data science methods have become indispensable in containing such an outbreak. The simple fact that significantly more data can be measured, analyzed, and understood, has profound implications in all of science and society.

5.2   Future Developments in Data Science

The data science vision is to measure more, to analyze more, and to know more. It is used in policy making: evidence-based-policy-making should lead to better decisions. It is used in policing: Intelligence-lead policing will reduce crime. Better data on consumer preferences allows marketers to create better recommendations and advertisements. More data allows astronomers to uncover more about our universe. By using large scale text analysis historians can better understand historical developments. The Internet of Things will cause a revolution in predictive maintenance. When the right information is available humanitarian aid can be more effective. New drugs can be discovered, outbreaks of diseases can be stopped, and diseases may eventually be eradicated, when the right information can be gleaned from the data.

Realizing this vision is dependent on science and technology. We must be able: (1) to have high quality data that can be represented and combined in a meaningful manner, (2) to analyze diverse and large data sets, and (3) to do so quickly, using high performance computing methods.

The goal of my chair is to create new data science methods, for the large and diverse data sets that scientists are increasingly using. Let us now look in more detail at the improvements that we will be working on. We will start with data quality and representation.

5.2.1   Data Quality & Representation

Open scientific data sources enable new forms of knowledge discovery. Publication mining experiments can yield results at significantly lower cost than traditional *in-vitro* experiments. The work in the field of knowledge representation, which studies taxonomies and information classification, is of great

importance here. At our center we are working on extending this to other sciences, for example to text mining of historical texts and to crowd sourcing for museum collections. Promising cooperations between biosemantics groups, database groups and high performance computing groups are happening.

We are in the fortunate position to have as part of our center one of the leading high performance database systems researchers, who works on MonetDB (Boncz et al., 2008). This is a great asset for all our data management research projects.

5.2.2   Analysis Techniques for Diverse & Large Data Sets

Advances in modeling drive statistical and computational techniques for Ebola, and for data science. An example is the need for validation of simulation results of multi-scale models (see, e.g., Portegies Zwart et al. (2013); Merks (2015)). The increased complexity of these models will demand better validation methods and lead to an increased need for observation data for initial values. In our center we are working on machine analysis of numerical simulation data, and on predictive maintenance. To compare the quality of algorithms benchmarks are needed. In machine learning we see benchmarking initiatives for data sets and algorithms, such as UCI[1] and OpenML.[2] We will use OpenML in our algorithm development work.

In many research projects a wide range of real world data is used from health (such as Ebola), to vibration data from bridges, to financial data from mortgages and commerce. LUMC, IBL and LIACS are working on knowledge representation and combinatorial optimization for metagenomics applications. Combinatorial algorithms are fruitfully applied in logistics operations in humanitarian aid, and many other scientific applications that have planning and scheduling challenges. In high performance combinatorial optimization a fundamental move to parallel algorithms has occurred, for example in high throughput drug discovery. This creates challenges for algorithm designers and a strong need for formal verification methods. I am looking forward to cooperation in this area.

At a more fundamental level, there is exciting work happening in search space analysis and visualization (see, e.g., Verbeek et al. (2007); Ochoa et al. (2014)), a possible combination with solution trees is interesting (Plaat et al., 1994a,b). We will look for relations between natural and heuristic optimization: finding common elements in evolutionary approaches (Bäck, 2014), deep

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[1]https://archive.ics.uci.edu/ml/datasets.html
[2]http://www.openml.org

neural nets (Krizhevsky et al., 2012; Van den Berg, 1996), pattern recognition, stochastic search (Kocsis & Szepesvári, 2006; Kuipers et al., 2013; Ruijl et al., 2014a), and classical enumeration algorithms (see, e.g., Russell & Norvig (2011); Ruijl et al. (2014a,b)). Recent experience with deep neural nets and stochastic optimization suggest the feasibility of such relations (see, e.g., Maddison et al. (2014); Clark & Storkey (2014); Mnih et al. (2015)). Also, genetic and evolutionary algorithms are often successfully applied to classic optimization problems (Izzo et al., 2013; David et al., 2014).

Such new methods will allow even more complex problems to be analyzed and understood. Many of the successes are driven by real world data and real world problems, such as the Ebola outbreak. Promising application areas are the analysis of simulation output, predictive maintenance, and drug discovery. Further application fields are humanitarian aid, marketing, organizational behavior and management (see, e.g., Plaat (2010)), financial analysis, and sports and, of course, health.

5.2.3   High Performance Computing

High performance computing in Leiden has a rich history in areas such as numerical computing, compiler technology, embedded systems, distributed computing, and sparse matrix codes with strong groups throughout the Faculty of Science. The work in the DAS projects (Seinstra et al., 2011), and the Little Green Machine[3] is state of the art. Data science needs a strong high performance systems group and we will work to further strengthen this field. Among the research topics are questions in compiler technology, data sharing (see, e.g., Kielmann et al. (1999); Plaat et al. (2001)), work and data scheduling (see, e.g., Romein et al. (2002); Kishimoto et al. (2013)), accelerators such as GPGPU (see, e.g., Mirsoleimani et al. (2014); Karami et al. (2014)), and other topics. Many applications, for example, imaging and astrophysics simulations, can benefit from these methods.

5.3   The Leiden Centre of Data Science

Scientists and society have found that high performance analysis methods can solve some of their problems and answer some of their questions. In fields ranging from the humanities, to astronomy, to containing outbreaks of contagious diseases, they learn more and create new insights.

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[3]http://www.littlegreenmachine.org

The purpose of the Leiden Centre of Data Science is to solve real world problems in science and society. In the process, these efforts drive the invention of new data science techniques. The interest in data science is high, inside our university, and outside. The Leiden Centre of Data Science is an ideal network organization for cooperation with other universities, academies, and data science centers. We cooperate with national and local governments, with commercial companies, and with social and cultural institutes. We organize data science summer schools, labs, and regular academic courses.

The purpose of the Centre is also to facilitate cooperation between different disciplines. As such our focus is on community building, on building a research infrastructure, and on initiating projects with researchers in academia and industry. Since the official opening of the Centre, less than a year ago, much has been achieved, and the interest in data science has only grown.

5.4 Conclusion

Mathematics and computer science are impacting our modern lives in many ways. The growing availability of data and data processing technology is causing profound changes in science and society: from the way that the Ebola outbreak is approached, to predictive maintenance of bridges and infrastructure, to fine grained marketing, to finding new drugs, to monitoring health behavior, to finding social networks in ancient Chinese texts, to analyzing computational fluid dynamics simulations, and to large scale simulations of star systems. Patterns are everywhere, and by learning to find them in large and diverse data sets we gain insights and solve problems.

From the perspective of data science the 2014 Ebola outbreak is of special significance. Governments and organizations provided open access to data, enabling the active creation of new data science tools. New diagnosis techniques and better epidemiological models have succeeded in reducing an aggressive epidemic faster than would otherwise have been possible. Pharmacologists are using high throughput methods that are increasing the chances of finding a vaccine. As a result, there is legitimate hope that this epidemic is soon under control. Data science is helping to save many lives—abstract notions from the worlds of statistics and algorithms are having an effect that is anything but abstract. The world is full of data, and data scientists are here to help.

At the start of this lecture I asked the question why there is so much interest in data. Subsequently, we discussed some important practical examples. Kurt Lewin once remarked that there is nothing so practical as a good theory, and I agree. For data science, such a theory has been proposed six years ago. In

2009 data-intensive research methods were named *the Fourth Paradigm* (Hey et al., 2009). This term implies that data science complements the methods of induction, deduction, and simulation, the three paradigms of the experimental cycle. The term suggests that data science is as fundamental as these scientific paradigms.

Data science gives scientists a new, disruptive, way to look for answers to their questions. For its consequences in theory and practice, we welcome data as a new paradigm to science.

Chapter 6

Acknowledgments

We have come to the end of this lecture. So, I would like to express my sincere thanks to the people who have been instrumental in the creation of this chair.

First of all, I thank the Board of Leiden University and the Board of the Faculty of Science for appointing me as professor of data science. I am grateful to the Boards, and in particular to Carel Stolker and Geert de Snoo, for supporting and creating the Leiden Centre of Data Science.

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Walle, I thank Meenal Pore from IBM Africa, and I thank Philips Research.

I thank my students, who have taught me so much. Science is a people's business, which is what I like about it so much (in addition to finding out new things, which is also very cool).

The last few words of this lecture are for three people, whom I value even above my love of science: Rosalin, Isabel, and Saskia. I thank you, with all my heart, for your love and laugther through all these years.

IK HEB GEZEGD.

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