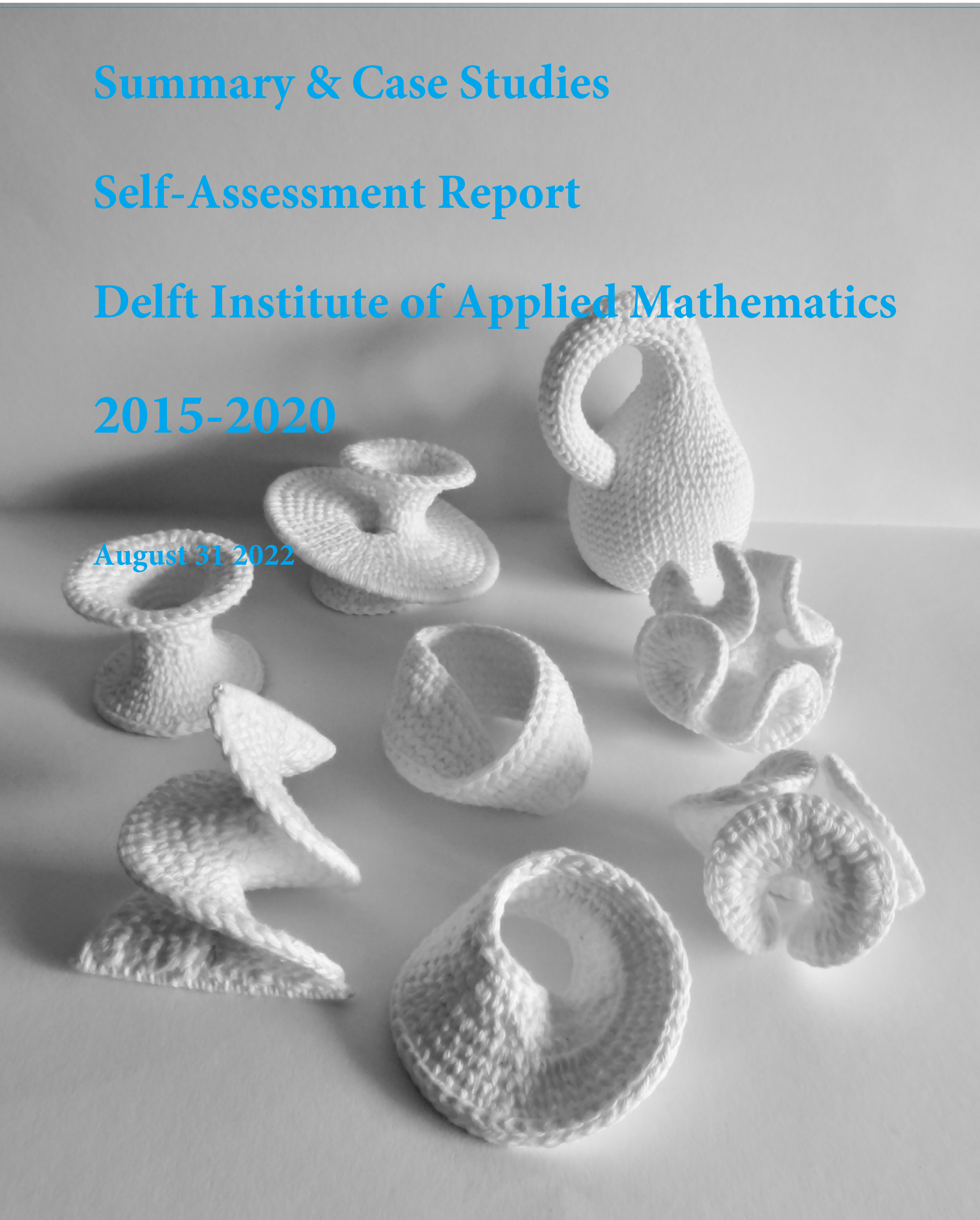
Summary & Case Studies

Self-Assessment Report

Delft Institute of Applied Mathematics

2015-2020

August 31 2022



Summary

Fundamental and applied problems in mathematics have become increasingly interwoven as the technological complexity of our society increases. DIAM's research scope covers all aspects necessary to address these mathematical challenges by developing theory and models.

Impact is made through publications in scientific journals; through education of the new generation of applied mathematicians and (via service teaching) engineers; and through collaboration with external partners. We consider our faculty members as our most important asset, and when hiring new staff our highest priority is to attract excellent candidates. Retention of faculty members is also of utmost importance. To this end, DIAM strives for a vibrant academic culture within the department, where there is sufficient research capacity for the department as a whole but also at the individual level. We also value diversity as a means to create a safe and pleasant working environment.

During the evaluation period, the number of faculty members at DIAM has increased. This led to a growth in research and teaching capacity for the department as a whole. However, because of the rise of the number of students at TU Delft, this has led to a consolidation of the research capacity of individual faculty members, rather than the increase desired.

DIAM members were successful in obtaining research grants from various sources. Personal grants, mainly VENI and VIDI grants, were acquired. For success with larger grants, two actions were undertaken. First, a more strategic approach to research funding was initiated, both for large scale thematic programs as well as personal grants. Second, focal research areas were identified to strengthen internal and external collaborations on these areas.

For the next six years, DIAM wants to further improve its academic culture and diverse working environment. Furthermore, we want to become leading in two major focal research areas: partial differential equations and mathematics of data science. This requires further improving cohesion within the department, organising conferences and taking leading roles in big projects. To facilitate this, we aim to support faculty members when they take leading roles in larger scale thematic projects. Support will also be provided for DIAM members when applying for personal grants.

Prof.dr. Kees Vuik
Head, Delft Institute of Applied Mathematics
Delft University of Technology

Case Studies

There are many axes along which research quality can be assessed. To give a more content-inspired impression of the work done at DIAM, this chapter includes six short narratives. These illustrate the range of DIAM's research in terms of sub-disciplines and vicinity to concrete fields of application.

In section 5.1, the societally highly relevant practical challenge of optimally positioning medical services is described. This illustrates DIAM's involvement in solving important societal problems. Section 5.2 addresses fundamental mathematical results related to quantum technology. This shows the connection of DIAM to research in this exciting domain, where TU Delft is a prominent player. In section 5.3, Bayesian networks are seen to be instrumental in describing the effect of task specialisation on the research careers of individual scientists. Section 5.4 exemplifies how DIAM's research helps air control to plan flights during volcano eruptions – specifically, how data assimilation (related to focal areas Partial Differential Equations and Mathematics of Data Science) helps in predicting the consequences of volcano eruptions, based on physical laws and measured data. Section 5.5 describes a simply formulated but notoriously challenging problem in terms of the card game SET that was finally settled. This fundamental research was published in the most prestigious fundamental mathematics journal, The Annals of Mathematics. Finally, section 5.6 highlights the importance of new numerical methods to make robust MRI scanners broadly available in developing countries, exemplifying the connection of DIAM's research to TU Delft's Global initiative.

Planning of Emergency Medical Services

In life-threatening situations, it is critical for emergency medical vehicles to arrive quickly. For the Netherlands, the target is that an ambulance should arrive at a scene within 15 minutes from the moment the call was made, in 95% of the cases. Failing to do so, can lead to a worsening of injuries, and in the worst case to loss of life. For the fire brigade and the police, similar response time targets exist. In this short overview we focus on ambulances.

There are two central questions to be addressed:

1. How many ambulance bases are needed to cover the demand within the given response time, and how many vehicles should be placed at each base? (Both the number of bases and number of vehicles can vary during the day.)
2. How can we, at any point in time, ensure coverage by dynamic repositioning of the available vehicles?

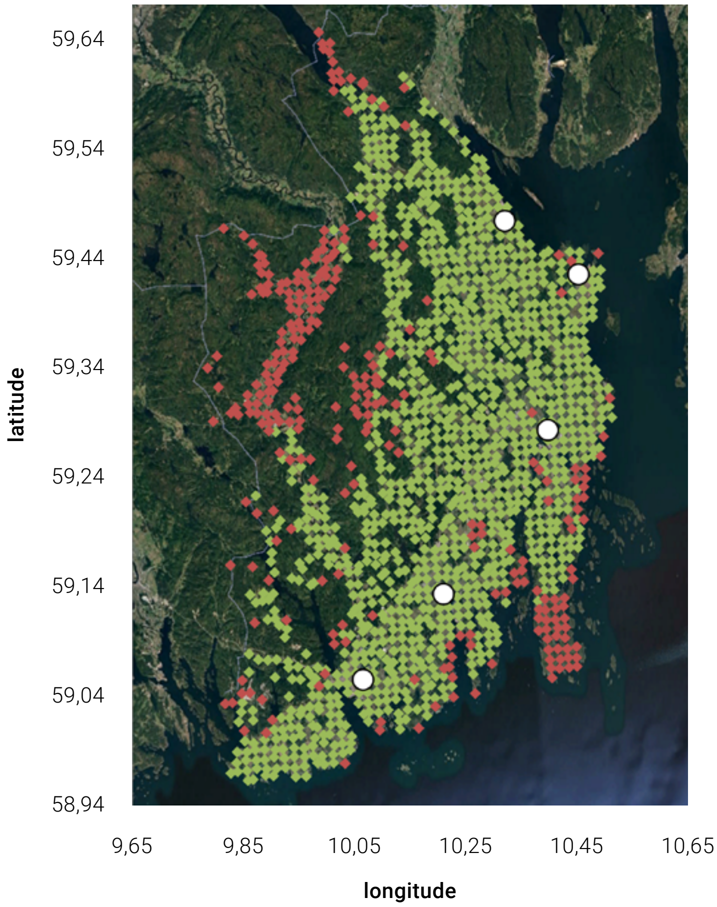


Figure 11: Positioning of ambulances in the region Vestfold, Norway. White circles are ambulance bases. Red/green areas the show uncovered/covered demand.

Determining ambulance bases

A useful starting point when determining the number of bases needed to cover the demand is the *Maximum Expected Covering Location Model*. Here, we want to maximise marginal coverage of the k-th ambulance, knowing the fraction of time an ambulance is unavailable due to a call. This so-called *busy fraction* typically varies substantially during the day. The model also requires as input a set of possible base locations, a set of demand points, travel times and demand at each demand point. At DIAM, we have investigated the following research questions. How can we best work with these models and their generalisations? What constitutes reasonable input? What are the effects of variations in the busy fractions, and the provided software for service providers such that they can see the effects of various changes in their data? An example of output[28] for a certain ambulance region in Norway can be viewed in Figure 11.

28 The picture is taken from P.L. van den Berg et al. 'Improving ambulance coverage in a mixed urban-rural region in Norway using mathematical modelling', PLoS ONE 14(4): e0215385. https://doi.org/10.1371/journal.pone.0215385.

Dynamic repositioning of vehicles

Given a fixed number of ambulances and a set of base locations, the other important problem to address is whether one can increase coverage by repositioning vehicles between bases. Suppose that a region loses coverage because the ambulance(s) that should cover the region are currently occupied. One could consider moving an ambulance from another region to restore that coverage. Moving a vehicle has consequences, of course, for the region where it was taken from, and can in turn initiate other movements. By designing an appropriate chain of movements, one can create more efficient usage of the available vehicles. This chain should of course only be initiated if the gain in coverage is above some threshold, since constant movement is disruptive for the crews. The call centre should also be able to maintain the overview.

Prof. Aardal, PhD student van den Berg and Dr. van Essen have cooperated with researchers at CWI Amsterdam, VU Amsterdam, The Norwegian Air Ambulance Foundation, Vestfold Hospital Trust, Norway, and with several safety regions in the Netherlands.

Simultaneous Quantum Mechanical Measurements

Quantum mechanics is the branch of physics that describes particles that are smaller than atoms. To describe the movement of such particles, new mathematical tools and models were designed a century ago, and these lead to stunning new opportunities in modern science, see Figure 12.

Krein's problem: uncertainty and perturbations of commutators

The quantum mechanical model exhibits two important features:

1. Measure outcomes are described by matrices and operators
2. The theory is probabilistic, yet cannot be understood by classical probability.

Both features are brought together in the famous Heisenberg uncertainty principle: measurement outcomes that are described by two non-commuting matrices cannot be determined simultaneously with full accuracy. In the quantitative form the uncertainty principle becomes:

$$\sigma(A)\sigma(B) \geq 2E[A,B]$$

Here, σ is the variance of measurement of matrices A and B which represent physical quantities like place and impulse. E is the expectation of the commutator $[A,B]=AB-BA$. The closer $[A,B]$ is to 0, the better A and B can be measured simultaneously.

In 1964, the renowned mathematical physicist M.G. Krein studied perturbations of commutators. For instance, one could add noise to a model or change variables A and B. Krein asked whether for self-adjoint matrices A and B and a suitable perturbation function f, we have

$$||[f(A),B]|| \leq c||[A,B]||$$

in some norm for some constant c.

If f is a polynomial, $f(A)$ is understood naturally; in general, we approximate f with polynomials.

Krein's problem has many applications in quantum mechanics and the analysis of functional calculus. However, the answer remained surprisingly shrouded in mystery for a long time.

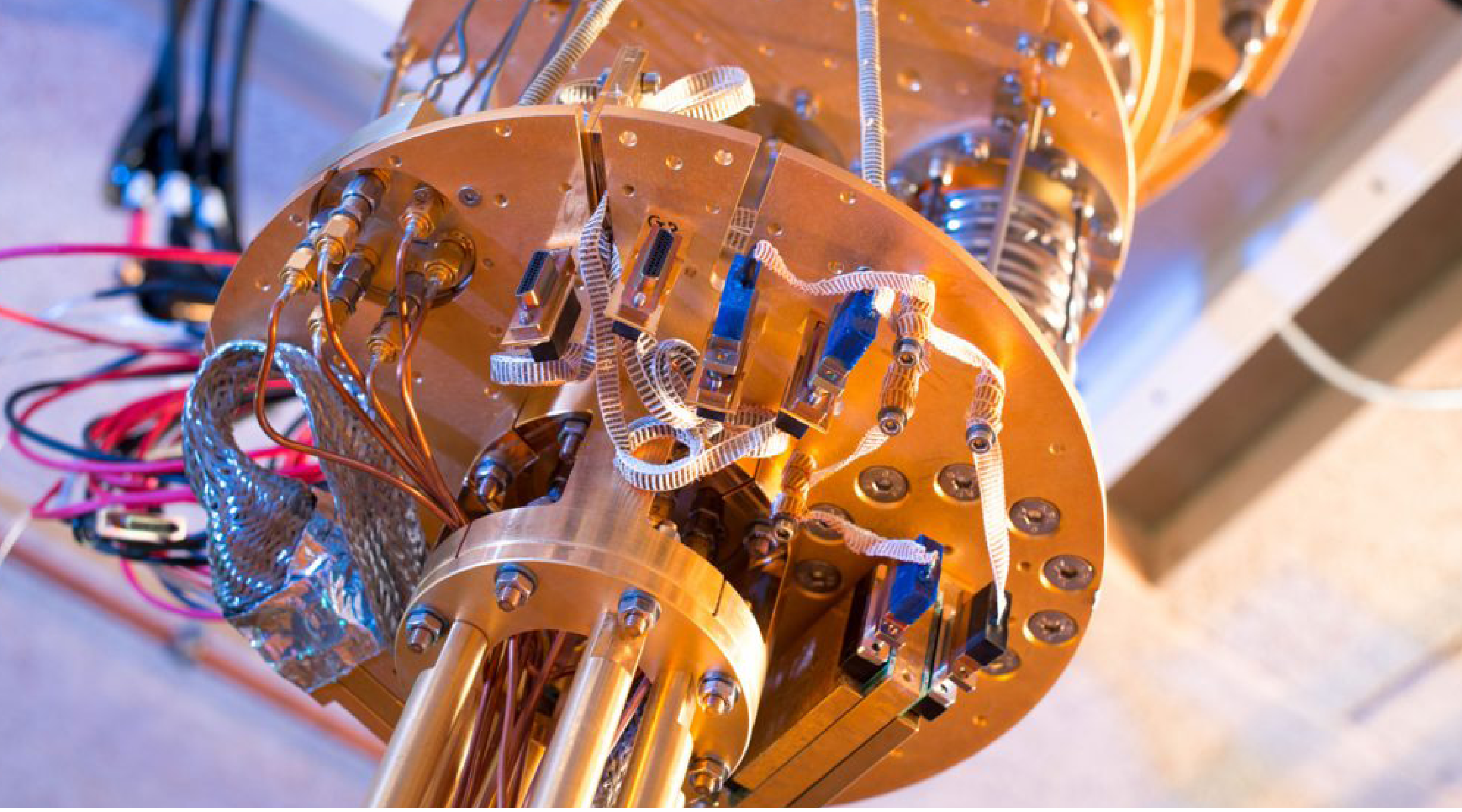


Figure 12: Uncertainty and error estimates play an important role in quantum computation at QuTech.

From quantum mechanics to modern harmonic analysis

Krein's problem was only resolved 50 years later by Fedor Sukochev and Denis Potapov at UNSW, Sydney. A solution remained elusive for such a long time because only at the start of the 20th century did the right tools from harmonic analysis came to the stage. A few years later, Dr. Caspers[29], now at DIAM, found sharp estimates for the constant c – now considered as the optimal solution to Krein's problem. To achieve this, several new tools have been developed in a new line of research called *non-commutative harmonic analysis*. Moreover, a whole range of problems was resolved using such tools, in both theoretical physics and mathematics.

Consequences of Task Specialisation for Research Careers

When a team of scientists conducts research and reports results in a publication, each researcher engages in different tasks, such as writing the paper (WR), conceiving the experiments (CE), performing the experiments (PE), analysing the data (AD), or contributing with analysis tools (CT). Researchers can engage in different tasks for the different publications they publish throughout their career. Research questions of interest include:

1. Do researchers engage in similar tasks for their publications?
2. Do the tasks researchers undertake change depending on their career stage?

29 Caspers' contributions to this area were awarded in 2018 with the Zemánek prize by the Polish Academy of Sciences for outstanding achievements in the area of functional analysis and operator theory under the age of 35.

During his Marie Sklodowska - Curie fellowship under the Leading Fellows program[30], Nicolas Robinson-Garcia[31] investigated the above research questions. Based on 70,694 publications in medical and life sciences, for which tasks have been reported for each co-author, Nicolas developed a Bayesian Network using task and bibliometric data. Bayesian Networks are probabilistic graphical structures that model dependent multivariate data. The five above mentioned types of tasks were considered. Bibliometric variables included document type, number of authors, countries and institutions for each publication.

The Bayesian Network was used to predict the tasks undertaken by 222,925 identified scientists for their complete publication history, which accounted to more than 6 million publications. The network demonstrated an impressive predictive performance, with at most an 8% classification error rate for all types of tasks.

Task specialisation

Nicolas' first observation was that, in general, researchers tend to engage in similar tasks for most of their publications. He identified what is known in the literature as task specialization. Nicolas used archetypal analysis to construct profiles of researchers. These are: *Leader*, characterized by high contributions to WR and CE; *Specialised*, with high contributions to PE and AD; and *Supporting*, with high contributions to AD and CT.

Career stage and length

To investigate the second research question, four career stages were considered: junior, early-career, mid-career and late-career. An archetypal analysis by career stage identified similar archetypes for each career stage. The vertical lines in the Sankey diagram[32] (Figure 13) show the proportion of researchers assigned to each archetype, for each career stage.

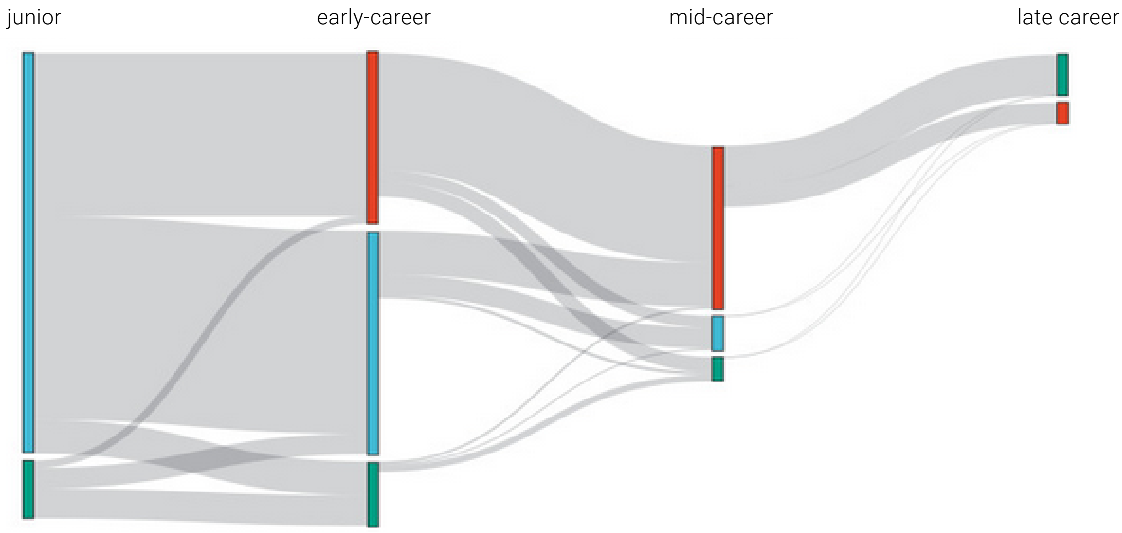


Figure 13: Sankey diagram showing the proportion of researchers assigned to each archetype for each career stage. Specialised profile (in blue); Supporting (in green); and Leader (in red).

30 https://leadingfellows.eu/

31 Under co-supervision by dr. Nane from DIAM, in collaboration with researchers from Centre for Science and Technology Studies (CWTS), Leiden University, Georgia Tech and Université de Montréal.

32 Robinson-Garcia, N., R. Costas, C.R. Sugimoto, V. Larivière, and G.F. Nane, 2020: Task specialization across research careers. **ELife**, **9**, 1-23.

Figure 14: Eyjafjallajökull volcano eruption plume.

The bands in the Sankey diagram show the evolution of individual researcher profiles through the entire career. The widths of the bands show the proportion of researchers who make it to the next career stage, by different profiles. As an example, a large cohort of Leaders in early career progress as Leaders in their mid-career (68.5%); 7% progress to a Specialised and 8.5% to a Supporting role, and 16% do not reach the mid-career stage.

Forecasting Volcanic Ash Clouds

Ten years ago, Europe was under the spell of an enormous ash cloud, following the eruption of the Eyjafjallajökull volcano on the Eyjafjalla Glacier in Iceland (see Figure 14). The cloud brought air traffic to a complete standstill in a large part of Europe, caused a great deal of disruption and entailed significant costs. DIAM PhD students Guangliang Fu and Sha Lu[33] investigated how such an ash plume behaves and how one can accurately predict where it will go. This is a subject that is extremely topical now that the Fagradalsfjall volcano on Iceland is restless. The mountain is spitting lava, ash and steam into the air, and volcanologists fear that a new and bigger eruption is imminent. More recently, the eruption of Cumbre Vieja on La Palma also stressed the relevance of this research project.

33 Under supervision of prof. Lin and prof. Heemink

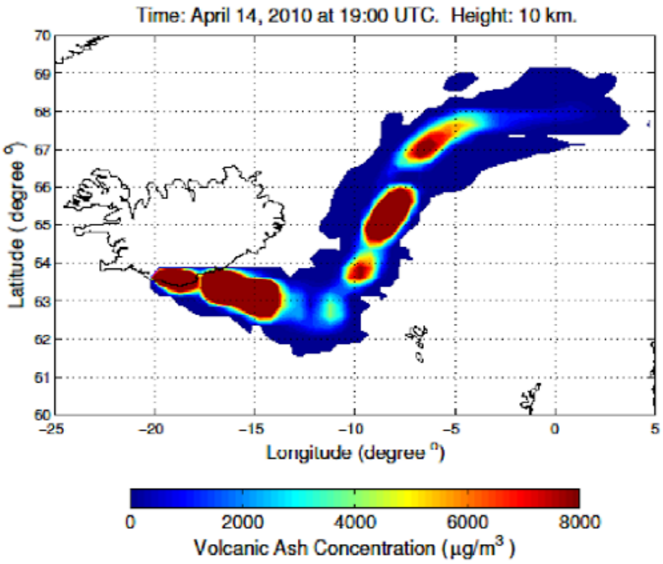


Figure 15: Modelled ash cloud, using data assimilation techniques.

Volcanic ash can cause serious damage to aircraft engines. Choosing to avoid any risks, airline companies decided to ground all of their planes. Knowing accurately where the ash cloud was headed could have made it possible to fly around it, and Guangliang Fu has successfully developed a model that is able to forecast ash cloud behaviour – priceless information for airlines and airports. Fu was one of the first to produce actual figures on ash cloud movement (see Figure 15). One of the reasons behind his success is the use of a detailed numerical model of the atmosphere that is combined with measurements from airplanes and satellites. The data assimilation algorithm that has been developed improves the model without violating physical conservation laws.

Satellite information alone does not offer a complete picture. Sending an aircraft to the cloud to conduct additional measurements is very effective. These data are also fed into his forecasting system. These measurements have no permanent location and that makes it more difficult to process the data.

Sha Lu conducted her PhD research into ash clouds at the same time as Fu. She explored algorithms that use satellite measurements for reconstructing the ash cloud at the site of the eruption itself, which would be beyond the capabilities of existing methods. A key question was where exactly did the ash enter the atmosphere, and what height did it reach? Lu looked at how to overcome the challenge posed by the fact that the satellites provide information only about the column as a whole, not the vertical distribution.' She combined these data with information from numerical models of the atmosphere, such as the wind speed at various altitudes.

Lu: 'Combining these data allows you to see how the ash is distributed vertically. It comes down to tiny differences that you have to extract from huge amounts of data. The information lies more or less concealed in a veritable mountain of data.'

Available inverse modelling algorithms were not able to handle this very ill-conditioned inverse modelling problem and Lu developed a new algorithm, trajectory-based 4D Var, to overcome this hurdle.

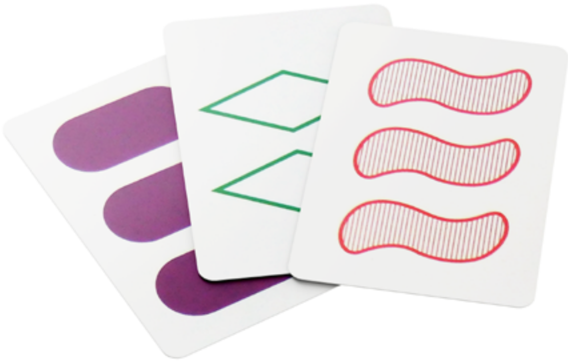


Figure 16: Card game SET.

Cutting-edge Combinatorics Inspired by a Card Game

The card game SET (Figure 16) consists of 81 cards made from four attributes that come in three flavours each. The simple goal is to find three 'matching' cards (a SET) that are the same or all-different for each attribute.

The question of how many cards you can have without containing a SET is a toy model for the so-called 'cap-set problem' in mathematics. Using a completely new set of tools, this problem was unexpectedly solved by Ellenberg (University of Wisconsin) and Gijswijt (DIAM)[34]. The result has direct implications for several areas in combinatorics and computer science.

Prof. Gijswijt: 'Ever since I was introduced to the card game SET as a student, I have been fascinated by the cap set problem. It is just a very beautiful mathematical question. Through the years I have often returned to this problem, mostly unsuccessfully. When a new idea in the so-called 'polynomial method' emerged recently, things finally clicked.' said.

What is the maximum number of cards you can have without creating a SET? The answer is 20, as was shown by the mathematician Pellegrino in 1971. This was three years before the game had been invented! His motivation for studying the problem came from the field of finite geometry.

Mathematically, the 81 cards from the game can be modelled as a 4-dimensional space, where each attribute corresponds to one independent direction. In this space, every line contains 3 points, and the lines are precisely the SETs.

Nothing stops us from considering spaces of dimension more than four. A set of points without any line is called a 'cap set'. The question of how large a cap set in n-dimensional space can be is called the 'cap set problem'. Field medallist Terence Tao suspected that this number would be $(3\text{-}o(1))^n$ and mentioned this in his 2007 blog post as one of his favorite questions. Others disagreed and conjectured that the density of a cap set would be exponentially small.

Mainly due to its connections to arithmetic progressions and certain problems in computer science, such as the sunflower conjectures and the quest for fast matrix multiplication, there has been a lot of interest in the problem in the last decades.

34 The results appeared in their N.G. de Bruijn prize winning paper in The Annals of Mathematics in 2017.

A breakthrough was obtained in 2012 by Bateman and Katz, who used sophisticated methods from Fourier analysis to show that the density of a cap set inside the whole space is less than the inverse of the dimension. However, this was still far from the conjectured exponentially small density.

By building upon very recent new ideas in the so-called polynomial method, Ellenberg and Gijswijt finally managed to settle this conjecture in the positive. One of the interesting features of the proof is the fact that it is very short.
Fields medallist Timothy Gowers in Quanta Magazine: '[The previous results] were already considered to be quite a big breakthrough, but this completely smashes the bounds that they achieved.'

The new proof methods (reformulated elegantly in terms of a new notion of `slice rank' by Tao), have already found many new applications in combinatorics. It will be exciting to see what other new mathematics is still in the cards.

Affordable MRI

High-field MRI scanners are commonly used in the West. In low- and middle-income countries, hospitals are simply unable to afford them. DIAM faculty member prof. van Gijzen is coordinator of an international team that develops a simple inexpensive MRI scanner based on permanent magnets for a children's hospital in Uganda (see Figure 17).

Figure 17. CURE children's hospital, Uganda.

Figure 18. Visit of Dutch project members to MUST, Uganda.

A simple MRI scanner can play a vital role in the diagnosis of hydrocephalus, a condition that affects over a hundred thousand children in sub-Saharan Africa. An early diagnosis can improve treatment, prevent severe brain damage, and save lives.

Van Gijzen's field is numerical linear algebra, or the algorithms behind technical applications and simulations. He deals with numbers and abstractions, and the implications of his work are often not immediately obvious to the outside world.

Van Gijzen: 'Writing a scientific article or developing an algorithm clearly matters to science but this project also has a much more direct social objective. It helps to find a solution to a major problem in the developing world, one that involves children as well.'

A normal MRI scanner has a superconducting magnet and liquid helium for cooling. It produces a complete, high-resolution picture. But scanners like this can cost up to three million euros and it takes highly specialised knowledge to operate and maintain them. Van Gijzen's aim is to develop a simple scanner which will cost no more than fifty thousand euros.

The use of a weak, permanent magnet instead of an expensive superconducting magnet leads to substantial savings, but it makes the mathematical side of things much more complicated and that is what Van Gijzen is working on with PhD students Merel de Leeuw den Bouter and Xiujie Shan and a number of MSc and BSc students.

Using a weaker magnet makes the results of the scans less accurate. To correct for this, several mathematical techniques can be used. The project studies methods to reduce noise and enhance edges in images based on nonlinear partial differential equations. The group also studies AI techniques to correct for image distortions and to improve image resolution. Using a combination of these techniques, they aim to improve the image quality sufficiently to aid in the treatment of hydrocephalus.

The project is a collaboration between TU Delft, Leiden University Medical Center, Pennsylvania State University (USA) and Mbarara University of Science and Technology (Uganda) (see Figure 18), and has received funding from STW through an Open Mind award, from NWO WOTRO, and from Delft Global Initiative. In addition to direct project partners there is also a collaboration with CURE children's hospital Uganda, and with the LDE center for Frugal Innovation in Africa.

'Using a weaker magnet makes the results of the scans less accurate. To correct for this, several mathematical techniques can be used.'