Exploratory experimentation in experimental mathematics: A glimpse at the PSLQ algorithm

Henrik Kragh Sørensen*

Institut for Videnskabsstudier, Aarhus Universitet, C. F. Møllers Allé 8, 8000 Århus C, Denmark

E-mail: hks@ivs.au.dk

1 Introduction

From a philosophical viewpoint, mathematics has traditionally been distinguished from the natural sciences by its formal nature and emphasis on deductive reasoning. Experiments—one of the corner stones of most modern natural science—have had no role to play in mathematics. However, in the past two to three decades, a mathematical subdiscipline has been forming that describes itself as "experimental mathematics", and it is the purpose of this paper to investigate and discuss the ways in which experimental mathematics is *experimental*.

Since the 1990s, many domains of knowledge production have witnessed a "computational turn" during which the wide use of computers has influenced established ways of thinking.[1] In mathematics, computers have been utilized since their first construction, but in the 1990s, their use led to a new subdiscipline of experimental mathematics in which computers were central to most—if not all—the experiments that give the subdiscipline its name. Using high speed computers and software packages such as Maple and Mathematica, mathematicians can now manipulate data and structures of immense complexity through real-time interaction with computers, and these practices are at the heart of experimental mathematics, I will argue. Thus, computers—and the "experiments" that they seem to carry with them—have entered into wide areas of traditional mathematics ranging from combinatorics to partial differential equations.

It is no coincidence that the name of the subdiscipline under consideration is often given as *experimental mathematics* or sometimes as *computer-based* or *computer-assisted* mathematics. Thus, it does *not* refer to a partic-

*The author wishes to thank participants at the conferences PhiMSAMP-3 (Vienna, May 2008) and ECAP-08 (Montpellier, June 2008), colleagues at the *Institut for Videnskabsstudier* (Aarhus), Jonathan Borwein (University of Newcastle, Australia), and two anonymous referees for valuable comments that helped shape and sharpen the argumentation in this paper.

[1]This "computational turn" was noticed also in the philosophy of knowledge, cf., e.g., (Burkholder, 1992, p. vii).

Benedikt Löwe, Thomas Müller (*eds.*). *PhiMSAMP. Philosophy of Mathematics: Sociological Aspects and Mathematical Practice*. College Publications, London, 2010. Texts in Philosophy 11; pp. 341–360.

Received by the editors: 28 September 2008; 19 May 2009.
Accepted for publication: 1 July 2009.

ular subject matter within mathematics, but rather to a specific technology (namely that of computers) and a specific, yet largely unspecified, methodology, namely that of *experimental* mathematics. The subdiscipline has consolidated itself around these two central notions with a set of key research questions and tools, a considerable infrastructure including journals and institutional embeddings,[2] and a philosophical legitimization brought about in articles and introductions to books such as *Mathematics by Experiment: Plausible Reasoning in the 21st Century* written by Borwein and Bailey (2004), two of the leading figures in experimental mathematics.

The philosophical literature on experimental mathematics and the discussions of computer-assisted mathematics have often revolved around a number of cardinal examples starting with the proof of the *Four Color Theorem* by Appel and Haken in 1976.[3] This prototypical example of a computer-based proof of a mathematical theorem involved computer-assisted 'number crunching' of a finite, but large, number of configurations to verify the claim. The admittance of such examples of 'number crunching' is discussed in the philosophical literature because they are perceived to involve a loss of surveyability that could challenge the *apriority* of mathematics.[4] Although these examples of 'number crunching' succeed in testing *all* the instances that fall under a general hypothesis, criticism can be levelled against them for not providing any *explanation* for the results obtained.[5] Another use of computers has been to perform searches within infinite domains in order to lend *inductive* support for a general hypothesis. An example of a distributed 'number crunching' of this sort is the search for huge *Mersenne primes*.[6] Similarly, the *Goldbach Conjecture* serves as a typical unsolved problem in number theory that has been subjected to immense 'number crunching' to establish that every even number less than 10^{18} can be written as the sum of two primes.[7] Hales' computer-assisted proof of

[2] Cf. (Gallian and Pearson, 2007, p. 14).

[3] Cf., e.g., (Tymoczko, 1979; Wilson, 2002; Bassler, 2006).

[4] Cf. (Bassler, 2006; McEvoy, 2008).

[5] Cf. also (Baker, 2007, 2008; Van Kerkhove and Van Bendegem, 2008; Van Kerkhove, 2005, pp. 287–307) and references in these for some of the themes of the discussion. The fact that 'number crunching' has an interesting history going back at least to the nineteenth century has been documented for the famous cases of the *Prime Number Theorem* (Echeverría, 1992), the *Goldbach Conjecture* (Echeverría, 1996), and *Fermat's Last Theorem* (Corry, 2008); cf. also (Goldstein, 2008).

[6] *Mersenne primes* are primes of the form $2^p - 1$. In September 2008, the distributed *Great Internet Mersenne Prime Search* (GIMPS) reported finding the 45th and 46th *Mersenne prime* each of which has more than 10^7 decimal digits.

[7] As of July 14, 2008, all even numbers less than 12×10^{17} have been verified to be expressible as the sum of two primes by the *Goldbach conjecture verification* project coordinated by Oliveira e Silva. The philosophical implications to be drawn from this form of inductive support for a mathematical statement has been discussed in, e.g., (Baker, 2007; Van Kerkhove and Van Bendegem, 2008).

the *Kepler Sphere Packing Problem* can be seen as a modern combination of these techniques, and it embodies most of the philosophical challenges posed by them.[8]

In the present paper, I go beyond these examples by bringing into play an example that I find more *experimental* in nature, namely that of the use of the so-called PSLQ algorithm in researching integer relations between numerical constants. It is the purpose of this paper to combine a historical presentation with a preliminary exploration of some philosophical aspects of the notion of experiment in experimental mathematics. This dual goal will be sought by analysing these aspects as they are presented by some of the protagonists of the field and discussing them using notions from contemporary philosophy of science.

Thus, in the following, I will introduce some of the most important philosophical discussions pertaining to experimental mathematics. I will then go on to illustrate how another feature of experiment may come into play in mathematics: namely that of exploration. In so doing, I describe a recent approach to experiments in science that focuses on their exploratory aspects and their importance in concept formation. Then, by combining this with a presentation of the PSLQ algorithm, I suggest to incorporate *experiments* in the informal portion of mathematics in a way that is loyal to mathematical practice while seeking to integrate the contexts of discovery and justification that are customarily separated.

2 Central themes: Induction and the role of computers

In 1998, when experimental mathematics was still in its infancy, Van Bendegem argued that mathematicians were using the term "experiment" in two essentially different ways, either as referring to computations or to real-world experiments. He found, that "it seems that it is very difficult to make any sense out of the idea of considering a computation (whether aiming for a numerical result or a visual image) as a form of mathematical experiment" (Van Bendegem, 1998, p. 178). A decade later, philosophical interest in experimental mathematics has only increased, and the impact of computers on traditional questions within the philosophy of mathematics is beginning to be investigated more. When Van Bendegem took up the philosophical analysis from (Van Bendegem, 1998) again together with Van Kerkhove, they noticed that experimental mathematics had "become established in [the] philosophical literature as an epistemic concept," (Van Kerkhove and Van Bendegem, 2008, p. 423) although the confusion over its precise meaning had still not been resolved. Consequently, they took up examples—some

[8] Cf., e.g., (Hales, 1994; Aste and Weaire, 2008).

of them exemplary ones—to discuss an "irreducible role in mathematics for genuine [as opposed to mathematical] induction (whether it be considered truly experimental or not)" (Van Kerkhove and Van Bendegem, 2008, p. 424).

In another recent paper, Baker continues the philosophical task of clarifying the meaning of experimental mathematics. First, he argues that "a literal reading of 'experiment,' in the context of clarifying the nature of experimental mathematics, is unfruitful" (Baker, 2008, p. 339). In particular, he questions whether computers are really *essential* to experimental mathematics and whether experimental mathematics is essentially about gathering inductive support for hypotheses. He finds flaws with both suppositions and instead suggests that the central feature of experimental mathematics is the calculation of instances of general hypotheses. However, Baker observes,

> [c]onfusingly, both computer use and inductive reasoning also have links to aspects of experimentation in science. What I [i.e., Baker] have argued, however, is that neither is an essential feature of experimental mathematics. There is experimental mathematics that makes no use of computers, and there is experimental mathematics that involves no inductive relations—claimed or actual—between evidence and hypothesis. (Baker, 2008, p. 343)

Surveying the field of computers in mathematical inquiry for an important recent volume on the philosophy of mathematical practice, Avigad also takes up the philosophical discussion of the role of computers in mathematics. Avigad's conclusion is that

> issues regarding the use of computers in mathematics are best understood in a broader epistemological context. [. . .] What we need now is *not* a philosophy of computers in mathematics; what we need is simply a better philosophy of mathematics. (Avigad, 2008, p. 315)

In particular, the use of the computer in mathematics and the impact it may have on so-called *experimental* mathematics needs to be described and understood within a framework sensitive to mathematical practice and to broader epistemological discussions.

Before I take up the discussion of these issues by extending and reshaping the notion of experiment, it is time to analyse the formation of the subdiscipline of experimental mathematics in the 1990s.

3 Experimental mathematics in the late twentieth century

Within the mathematical community, experimental mathematics became a debated topic in the 1990s, when the *American Mathematical Society* (AMS) and its journals devoted resources to discussing the implications of computers for mathematics. In retrospect, a column on "Computers and Mathematics" run in the *Notices of the AMS* from the summer of 1988 to the end of 1994 may be seen as the immediate context of experimental mathematics in the form discussed here (Devlin and Wilson, 1995, p. 248). Among reviews of software packages and technical results, some discussions evolved around visions of the impact of the computer (and digital storage and correspondence) for the communication of mathematical results—and conjectures. In connection with this, a perceived loosening of the standards of rigour was also discussed in the context of the enormous potential of the computer. In 1993, this discussion hit the mathematical community with force when Jaffe and Quinn published their suggestion for a separation between two branches of mathematicians, one that was *speculative* and one that was *rigorous*.[9] Among the debaters, it was argued that the mathematical community should be *inclusive* when it came to computers. From a variety of points, mathematicians argued that mathematics ought to embrace computers, even if this would lead to changes in the means of doing and communicating mathematics, although any loosening of epistemic standards was hard to accept for most. These issues since became important for discussions of experimental mathematics.

In the mainstream views, experiments could be useful as *heuristics*, but according to these deductivist and formalist conceptions of mathematics that Lakatos has identified as the *Euclidean myth*, such heuristics were confined to the informal spheres of discovery and teaching. Most certainly, they could not be allowed to aspire to anything like the status of proof. To these mathematicians, deductive proof is the exclusive mode of knowledge production in mathematics. However, in the 1990s, a new wave of "experimental" mathematicians was about to challenge these views.

The number of mathematicians actively identifying themselves with the new experimental programme in the early 1990s was rather limited, as would be expected. But soon, it came to associate also with prominent mathematicians such as Fields-medalists Thurston, who has a strong interest in the impact of computers on mathematics.[10] Despite its size, the group of experimental mathematicians was a heterogeneous one. Individuals committed to experimental mathematics held differing conceptions of the scope of experiment, and in particular of the kind of use that computers could

[9] (Jaffe and Quinn, 1993); cf. also (Atiyah et al., 1994; Jaffe and Quinn, 1994). Taking their lead from the division of labour within physics, Jaffe and Quinn used the terms "theoretical" and "rigorous". However, as used, I find that what they called "theoretical" is better captured under the heading "speculative"; cf. also (Thurston, 1994, p. 163).

[10] (Bown, 1991). Thurston had received the Fields medal in 1980 and was recognized as a leading figure within the mathematical community in the 1990s. Cf. also (Thurston, 1994) for Thurston's reactions to Jaffe and Quinn and (Horgan, 1993) for some of the controversy involved in the issue at the time.

be put to in experimenting with mathematics. One cluster formed around the journal *Experimental Mathematics* when it was founded in 1991 and began appearing the following year with Epstein and Levy as editors (Epstein and Levy, 1992). A different cluster formed in Canada at *Simon Fraser University* around a group of individuals including J. M. Borwein, P. Borwein, and Bailey. In geographical proximity and sharing a common research agenda and a powerful set of computer routines and algorithms, this group institutionalised as *Centre for Experimental and Constructive Mathematics* (CECM) in November 1993. A third group to be mentioned here centers around Zeilberger whose research programme is related to that of the CECM-group but exhibits some remarkable philosophical differences.

4 Experimental mathematicians philosophizing

The protagonists of experimental mathematics have been quite explicit about the philosophical problems involved in their line of mathematical research. In a central article in the early history of experimental mathematics, "Making Sense of Experimental Math" (published in the *Mathematical Intelligencer* in 1996), the brothers J. M. Borwein and P. Borwein and two collaborators describe the new field, its possibilities, and its challenges (Borwein et al., 1996). They offer the following definition of the field drawn from a characterization of four roles of scientific experiments given by the philosophizing immunologist Medawar (1979):

> *Experimental Mathematics* is that branch of mathematics that concerns itself ultimately with the codification and transmission of insights within the mathematical community through the use of experimental (in either the Galilean, Baconian, Aristotelian or Kantian sense) exploration of conjectures and more informal beliefs and a careful analysis of the data acquired in this pursuit. (Borwein et al., 1996, p. 17)

This definition emphasises the changes in infrastructure required for a shift towards more experimental methods in mathematics. In other (later) publications, the same authors expand on the particular roles for the use of computers in mathematics (Borwein and Bailey, 2004, pp. 2–3), as they see the "utilization of modern computer technology as an active tool in mathematical research" in the style of experimental mathematics (Bailey and Borwein, 2005, p. 502). The role of computers in mathematical experimentation will include (cf. Figure 1) *heuristics* [1–3] (gaining insight and intution and discovering new patterns using symbolic or graphical experiments), *refining and evaluating conjectures* [4–5] (testing and falsifying conjectures and exploring the conjecture to see if it is worth attempting a formal proof), and *aiding in the procedure of proving conjectures* [6–8], either by suggesting strategies for formal proof or by allowing computer-based derivations or confirmations of, e.g., intricate identities (Borwein and Bailey, 2004, pp. 2–3).

1. Gaining *insight and intuition.*
2. *Discovering new patterns* and relationships.
3. Using graphical displays to *suggest underlying mathematical principles.*
4. Testing and, especially, *falsifying conjectures.*
5. Exploring a possible result to see if it is *worth formal proof.*
6. *Suggesting approaches* for formal proof.
7. Replacing lengthy hand derivations with *computer-based derivations.*
8. *Confirming* analytically derived results.

FIGURE 1. Roles for computers in mathematics, according to (Borwein and Bailey, 2004, pp. 2–3).

Among the types of experiments extracted from Medawar's classification, "Baconian experimentation" includes "trying things out" and observing "things as they really are" (Medawar, 1979, pp. 69–70). This type of experimentation could seem to come close to the use of computers in visualizing and exploring mathematical structures and problems. However, compared to Medawar's four types of scientific experiments, the authors argue, experimental mathematics is only a "serious enterprise" insofar it resembles the critical (or even crucial) experiments that Medawar calls "Galilean" which "discriminate between possibilities and, in doing so, either gives us confidence in the view we are taking or makes us think it in need of correction" (Borwein and Bailey 2004, p. 6; cf. also Medawar 1979, p. 71). Although superficial, Medawar's presentation of Baconian experiments highlights their ideal characteristic as unbiased recordings of contrived facts of nature that can subsequently be subjected to inductive arguments. Thus, the authors contrast the *inductive* Baconian experiments with the crucial, and thereby essentially *deductive*, experiment that Medawar ascribes to Galilei. By their emphasis on the latter, these authors therefore also argue for a deductive and justificatory role for experiments in mathematics that goes beyond the heuristics of fact (number) gathering.

However, as I will discuss below, I find that the discussions of so-called "new experimentalism" and the notion of "exploratory experimentation" bring a new and refined meaning to Baconian experimentation that has consequences for the understanding of mathematical experiments (Steinle, 1997).

5 Contexts of experiments in the sciences and in mathematics

In the second half of the twentieth century, a standard view of the role of experiments in the sciences has been to test hypotheses or theories. Such *theory-driven* experimentation resembles Medawar's Galilean experiments and serves to justify theories. In mathematics, on the other hand, experimentation has been accepted as a (powerful) heuristic that can aid in the *discovery* of plausible conjectures. But, in mathematics, experiments have been confined to the realm of discovery while deductive *proofs* remained the exclusive means for justifying claims in mathematics.

What has happened in the past decades has been that these opposite confinements for experimentation have begun to be loosened in the philosophical literature. In the sciences, "exploratory experimentation" has been analysed as an important means of concept formation. Thus, experiments in the sciences have found a place in the context of discovery together with the heuristic of gathering data. In mathematics, where experiments were typically confined to the context of discovery, experiments have started to blur the distinction in the other direction. Some proponents of experimental mathematics—in particular Zeilberger—have claimed that experiments possess powers of justification that are not those of proofs, but could and should be allowed into mathematics. Thus, the notion of experiment is changing both in the sciences and in mathematics, but because the traditional views differ in science and mathematics, the new roles for exploratory experimentation also differ.

Thus, when the concept of experimental mathematics made its dramatic entry onto the scene of the mathematical community in the first half of the 1990s, the image of experimentation, itself, was undergoing refinement in the philosophical literature.[11] In the following, I suggest that "exploratory experimentation" offers a framework for understanding some of the epistemological claims of experimental mathematics.

[11] Cf., e.g., (Steinle, 2002, 1997; Franklin, 2005).

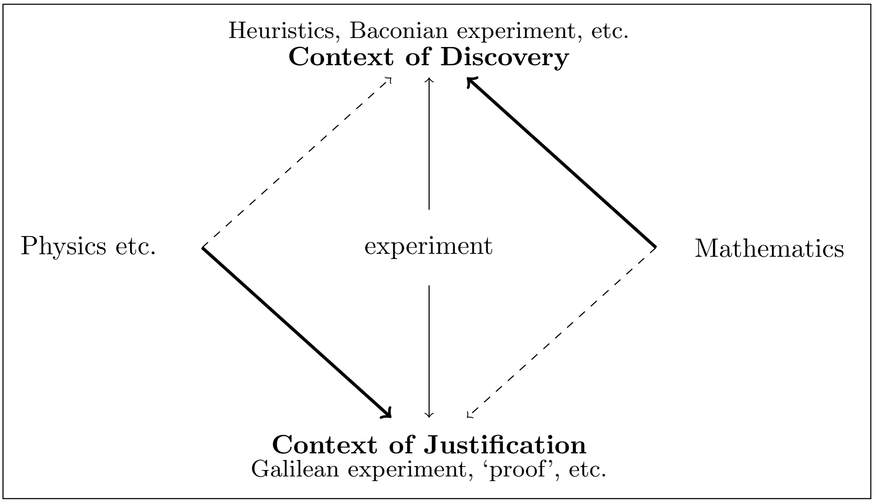

FIGURE 2. The uses of experimentation is changing both in the sciences and in mathematics. The thick arrows indicate traditional embeddings of experiments in science (justification) and mathematics (discovery). The dashed arrows indicate new roles for experiments, and the vertical arrows are meant to indicate that changes in the notion of experiment are blurring the distinctions between the contexts of discovery and justification. Importantly because the traditional views of the two types of science are different, the new roles for exploratory experiments also differ.

6 Exploratory experimentation and wide instrumentation

The philosopher of (physical) science Steinle describes the differences between theory-driven and exploratory experimentation in terms of the possible empirical outcomes:

> Theory-driven experiments are typically done with quite specific expectations of the various possible outcomes in mind. [...] Exploratory experimentation, in contrast, is driven by the elementary desire to obtain empirical regularities and to find out proper concepts and classifications by means of which those regularities can be formulated. (Steinle, 1997, p. S70)

Steinle goes on to explain that exploratory experimentation typically takes place in phases of scientific development in which no well-formed conceptual framework is available (Steinle, 1997, p. S70). Thus, Steinle's exploratory experiments in science are *open-ended* and highly important and influential in the processes of concept formation.

Drawing on examples from research in molecular biology during the last decades, the philosopher Franklin adds an interesting dimension to the notion of "exploratory experimentation", namely that of *wide instrumentation.* The availability of high-throughput instruments that can simultaneously measure many features or repeat measurements very quickly has, so Franklin argues, made it feasible (again) to address the enquiry of nature without local theories to guide the experiments. In the process, experiments have gained another quality to be measured by, namely efficiency in bringing about new results (Franklin, 2005, p. 895).

These aspects of exploratory experimentation and wide instrumentation originate from the philosophy of (natural) science and have not been much developed in the context of experimental mathematics. However, I claim that, e.g., the importance of wide instrumentation for an exploratory approach to experiments that includes concept formation also pertain to mathematics. However, it could seem that experimental situations with no well-formed conceptual framework do not occur in mathematics. Therefore, I first give a short outline of an example to illustrate that this can and does occur. I then go on to discuss the idea of exploratory experimentation based on another example from experimental mathematics, namely the so-called PSLQ algorithm.

7 In the absence of a well-formed conceptual framework

Experimental mathematicians have taken an interest in studying polynomials with coefficients from a finite set. For instance, a group at the CECM has studied zeroes of polynomials with coefficients 1 or -1 and degree up to 18.[12] Extensive data mining was used to produce graphical illustrations of the sensitivities of the zeroes of these polynomials. From these images, two observations can be made that are important in relation to Steinle's notion of exploratory experimentation. One point is that the images were found to exhibit a remarkable behaviour near roots of unity, and indeed, that behaviour has now been rigorously proved (Borwein et al., 2008). The other point is that the images were capable of interactive experimentation such as measuring sensitivities relative to one of the coefficients. Figure 3 illustrates the sensitivities of zeroes relative to the x^9 term. These new figures, and in particular the banded features that appear, are not yet fully understood. However, it is widely believed among the experimental experts that the features are stable and not merely programmatic artifacts. To understand these new phenomena, it is most likely that some new conceptual

[12] Polynomials with coefficients ± 1 are called *Littlewood polynomials.* This example and Figure 3 below is presented in (Borwein and Jörgenson, 2001) and briefly described in various publications on experimental mathematics, such as (Borwein, 2008).

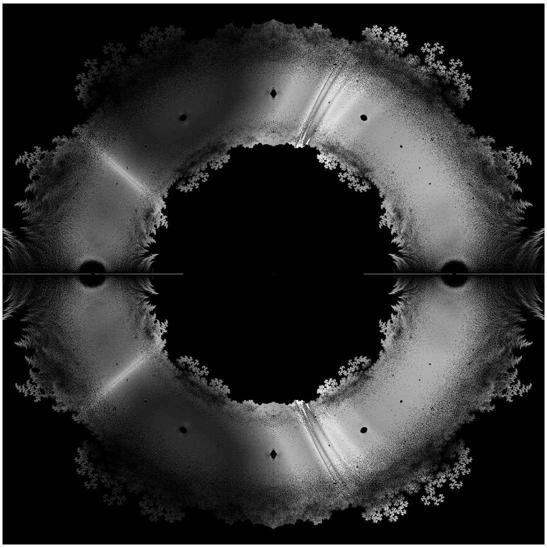

FIGURE 3. Sensitivies of zeroes of *Littlewood polynomials* of degree up to 18 relative to the x^9 term; image from Loki Jorgensen's webpage.

developments are required. Thus, this is a case in which computer-assisted methods—both in the form of data mining (or 'number crunching') and as open-ended, exploratory and interactive experimentation—are at work in a situation when no well-formed conceptual mathematical framework for explaining the phenomena has yet been devised. A variation on this situation will appear below in the case of the PSLQ algorithm.

8 The PSLQ algorithm as an example

The group of experimental mathematicians centred around the CECM and the brothers J. M. Borwein and P. Borwein have made use of an algorithm developed by Ferguson, Bailey and others, known as the PSLQ algorithm.[13] This algorithm is a good example of a powerful tool in experimental mathematics and therefore merits some attention and analysis in the present context. First, the domain of the algorithm needs to be clarified. The PSLQ algorithm is a so-called "integer relation detection algorithm" that can be used to search for integer relations between given numerical constants expressed in finite, but high-precision decimal representation. By a special application, the PSLQ algorithm can also be used to investigate

[13] (Ferguson et al., 1999). The PSLQ algorithm has also been discussed in (Corfield, 2003, pp. 64–66).

whether given numerical constants are algebraic numbers or not. Thus, the algorithm has found its use, e.g., in summing various series in closed form (Bailey et al., 1994). Second, the special nature of the PSLQ algorithm that makes it *experimental* needs to be emphasized. The algorithm takes as its input a vector of high-precision real (or complex) numbers $(x_1, \ldots, x_n) \in \mathbb{R}^n$ and after a bounded number of iterations either produces 1) a vector of integers $(m_1, \ldots, m_n) \in \mathbb{Z}^n \setminus \{0\}$ such that the linear integer combination $\sum_{k=1}^{n} m_k x_k$ is very close to zero with high precision, or 2) a lower bound R such that for all vectors of integers bounded by R, the linear integer combination $\sum_{k=1}^{n} m_k x_k$ is provably different from zero. The two potential outcomes of the algorithm, therefore, represent an unproven suggestion or a provable non-existence result: The result is either a suggestion for an integer relation or a lower bound showing that any such relation has to include very large coefficients.

9 Consequences and applications of the PSLQ algorithm

In case the PSLQ algorithm provides a lower bound for the size of any possible integer relation between the specified real constants, the result is exact (and provable). However, the community of experimental mathematicians have come to hold different—some of them rather radical and provocative—views on the need for making the proof explicit. The most outspoken radicalist among them, Zeilberger, has suggested that when such exact results are provided by an established algorithm, it suffices to annotate the announcement with “QED” as a seal that the author has, indeed, performed the computation and observed the result as indicated.[14] In some of his papers and preprints, of which his software package “Ekhad” is listed as co-author, Zeilberger has even implemented this (cf. Figure 4).[15] The provocative nature of the views of the most radical experimentalists in mathematics is even clearer when it comes to the status of a result such as an output of the first type from the PSLQ algorithm: a statement of a high-precision verification of some relationship. Following up on a provocative suggestion by Chaitin and in line with some of the arguments behind the suggestions of a “theoretical mathematics” discussed above, Zeilberger has suggested to affix statements of this kind with a (consistently derived) estimate of how difficult or time-consuming it would be to produce a formal proof of a relationship that is verified to great numerical precision.[16]

What lies behind Zeilberger’s suggestion is that mathematics is presently in a phase of wide expansion, cultivating ‘new lands’. During such a phase,

[14] Cf., e.g., (Zeilberger, 1993, p. 31).
[15] Cf., e.g., (Ekhad and Zeilberger, 1996).
[16] For Zeilberger’s elaboration, cf. (Zeilberger, 1994).

> *Proof.* While this is unlikely to be new, it is also irrelevant whether or not it is new, since *such things are now routine, thanks to the package* ***qEKHAD***, accompanying [PWZ]. Let's call the left side divided by $q^{m(m-1)/6}$, $Z(m)$. Then we have to prove that $Z_0(m) := Z(3m)$ equals $(-1)^m$, $Z_1(m) := Z(3m+1)$ equals $(-1)^m$, and $Z_2(m) := Z(3m+2)$ equals 0. It is directly verified that these are true for $m = 0, 1$, and *the general result follows from the second order recurrences produced by* ***qEKHAD***. The input files `inZ0`, `inZ1`, `inZ2` as well as the corresponding output files, `outZ0`, `outZ1`, `outZ2` *can be obtained by anonymous* ***ftp*** to `ftp.math.temple.edu`, directory `pub/ekhad/sasha`. The package `qEKHAD` can be downloaded from `http://www.math.temple.edu/~zeilberg`. Q.E.D.

FIGURE 4. A "proof" according to Ekhad and Zeilberger in the *Electronic Journal of Combinatorics*, (Ekhad and Zeilberger, 1996, p. 2, emphasis added).

efficiency in establishing results is to be valued more, they think, than absolute rigor according to the traditional standards. Therefore, Chaitin has suggested assuming unproved hypotheses such as the Riemann Hypothesis as axioms if they are experimentally justified and lead to fruitful research.[17]

Unsurprisingly, Zeilberger's suggestion was met with criticism from proponents of a more classical view of mathematical epistemology.[18] The CECM-group also takes a different view of the situation. As the nicely titled paper "Strange Series and High Precision Fraud" argues (Borwein and Borwein, 1992), even high-precision verification is *not* a substitute for formal proof.

Although the field of experimental mathematics is considerably broader than applications of the PSLQ algorithm and similar searches for symbolic identities using numerical methods, the PSLQ algorithm is a nice example from which to discuss features of the new experimental approach to mathematics. Integer relation detection is located on the border between rigorously provable theorems and experimentally obtained conjectures. The PSLQ algorithm allows mathematicians to interactively navigate open problems in many fields of mathematics in search of either rigorous lower bounds or suggestions for relations. If the algorithm provides a rigorous lower bound, mathematicians may continue pursuing a proof that no such relations exist at all. On the other hand, if the algorithm suggests a relation,

[17]Cf., e.g., (Chaitin, 1993, pp. 326–327).
[18]Cf., e.g., (Andrews, 1994).

mathematicians may seek traditional proof of this suggestion. In both cases, the situation is likely to be further explored using either experimental techniques or more traditional proof, or a combination thereof.

10 Fact-gathering or interactive exploration

A traditional (post-foundationalist) framework for discussing the philosophy of mathematical practice has been Lakatos' conception of mathematics as a quasi-empirical science directed by thought-experiments (also known as proofs) and refutations through counter examples (Lakatos, 1976). Thus, Lakatos' philosophy as expressed in the *Proofs and Refutations* deals mainly with concept formation presupposing phases of heuristic conjecturing. If Lakatos' philosophy is to be fully applied, another aspect of experimental mathematics has to be considered. Gauss' calculations (with the help of *human* computers) of prime number tables to a large extent fell into the category of fact-gathering for subsequent conjecturing. As such it can be isolated as a most fundamental form of experiment, but not (yet) as exploratory experimentation. Similarly, many of the efforts that have gone into computer visualisation and 'number crunching' of mathematical problems have served these roles of compiling and making accessible data on which to form hypotheses. However, the interactive use of systems such as Maple and Mathematica have opened the door for an integrated process of experimentation, concept formation, and conjecturing. This can be illustrated using an example relating to so-called *Euler sums* and using the PSLQ algorithm that has been discussed by members of the CECM-cluster in (Bailey et al. 1994; cf. also Borwein et al. 1996, pp. 13–15).

As recorded in (Borwein et al., 1996, pp. 13–15), an undergraduate student observed the curious numerical fact that

$$\sum_{k=1}^{\infty}\left(1+\frac{1}{2}+\cdots+\frac{1}{k}\right)^2 k^{-2} = 4.59987\cdots \approx \frac{17}{4}\zeta(4) = \frac{17\pi^4}{360}$$

and brought it to the attention of his professor (J. M. Borwein). At first a serendipitous discovery, the experimental mathematicians began to explore the relationship to greater numerical precision. When the relation was confirmed to a precision of 100 digits, they undertook to generalise the setting and produce a framework for experimentally exploring similar conjectures using the PSLQ algorithm. Among many similar so-called *Euler sums*, they investigated sums of the form

$$s_a(m,n) = \sum_{k=1}^{\infty}\left(1-\frac{1}{2}+\cdots+\frac{(-1)^{k+1}}{k}\right)^m (k+1)^{-n} \quad \text{for } m \geq 1, n \geq 2$$

and

$$s_h(m,n) = \sum_{k=1}^{\infty} \left(1 + \frac{1}{2} + \cdots + \frac{1}{k}\right)^m (k+1)^{-n} \quad \text{for } m \geq 1, n \geq 2.$$

These new expressions are thus part of a conceptualisation introduced in order to formulate and generalise the outcomes of exploratory experimentation.

The integer relation detection of the PSLQ algorithm functioned as an important tool in finding potential integer relations involving other known mathematical constants. When such relations are found using high precision computations, the experiment is concluded, and it may either (according to Zeilberger's view) be accepted as an experimentally derived and supported result, or be subjected to formal proof. For some of the many identities obtained by Bailey and his coauthors, formal proofs have been found, whereas others remain open conjectures. For instance,

$$s_h(2,2) = \frac{3}{2}\zeta(4) + \frac{1}{2}\zeta^2(2) = \frac{11\pi^2}{360}$$

has been formally proved (1996), whereas

$$s_h(3,2) = \frac{15}{2}\zeta(5) + \zeta(2)\zeta(3)$$

remained a conjecture (1996). As part of the process of exploratory experimentation, new connections between various constants (and, therefore, presumably between various sets of theories) are suggested and need to be explored.

Experimental mathematicians repeatedly stress the importance of *interactive* experimentation using computers, for which high-speed processors as well as a functional user interface is imperative. For this, they often profess their debt to *Moore's Law* that semiconductor performance doubles every 18 to 24 months.[19] In doing so, they repeat some of the arguments for wide instrumentation discussed by Franklin. Only with interactive experimentation and multi-purpose software—so it seems—could mathematical experimentation make a transition from 'number crunching' to exploration. Thus, high-speed computers and interactive software packages seem to be the mathematical equivalents of wide instrumentation in the sciences. In particular, this suggests an answer to why experimental mathematics *only* became a discussion in the 1990s when both hardware and software had been developed to meet these demands.

[19] Cf., e.g., (Borwein and Bailey, 2004, pp. 3–4). However, for the notion of *Moore's Law* and technological determinism, cf. (Ceruzzi, 2005).

Thus, perhaps as a result of not referring to the most recent literature that includes exploratory experimentation, experimental mathematics has so far missed out on an obvious and yet very powerful symmetry with the use of experimentation in the sciences. It is becoming increasingly clear that experiments have an important role in the concept formation in the sciences—a realization that is a reaction to the exclusive focus on theory-driven experiments in much of the twentieth century. Similarly, an important role is to be played by computational experimentation in mathematics, when it is performed in the interactive, exploratory ways discussed above.

11 Is (experimental) mathematics special?

This paper has described aspects of the emerging discipline forming around the use of computer experimentation in mathematics and institutionalising as experimental mathematics. This subdiscipline has challenged the usual deductivist philosophy of mathematics by arguing for a role for experiments in mathematics. Thereby, its proponents not only blur the separation between the context of discovery and the context of justification in mathematics but also claim a role for experiments beyond that of heuristics.

By way of a single example—that of the PSLQ algorithm—I have shown how the methodology of experimental mathematics features examples of exploratory experimentation similar to the kind recently discussed in the philosophy of the sciences. Thereby, I have pointed out that the practice of experimental mathematics is, indeed, experimental in some of the ways most often associated with physics or chemistry.

On the other hand, even within the community of experimental mathematics, views differ concerning the role of experiment in justifying mathematical claims. They all claim a role for it, but differ on precisely which one. Here, again, I see a role for exploratory experimentation as a framework. It highlights the role of experiments in the process of concept formation that can lead to (formal) theory formation. In these respects, therefore, experimental mathematics *does* pose an example challenging traditional views of mathematical epistemology and bringing forward a suggestion for a more empirically founded philosophy of mathematics that applies, at least, to the domains of mathematics most susceptible to exploratory experiment.

To finally address the question whether (experimental) mathematics is special, I would point out, that even considering exploratory experimentation, "experiment" still means essentially different things in the sciences and in experimental mathematics as was pointed out by, e.g., Baker (2008) in the introduction. However, the emergence of experimental mathematics shares features with exploratory experimentation in the sciences, particularly when it comes to open-ended experimentation, wide instrumentation, and the role of experimentation in concept formation. Thereby, this suggestion raises (again)—and from the novel perspective of comparing with the sciences—the question whether deductive proof is *really* the only permissible mode of justification in mathematics.

Bibliography

Andrews, G. E. (1994). The death of proof? Semi-rigorous mathematics? You've got to be kidding! *The Mathematical Intelligencer*, 16(4):16–18.

Aste, T. and Weaire, D. (2008). *The Pursuit of Perfect Packing.* CRC Press, Boca Raton FL.

Atiyah, M., Borel, A., Chaitin, G. J., Friedan, D., Glimm, J., Gray, J. J., Hirsch, M. W., MacLane, S., Mandelbrot, B. B., Ruelle, D., Schwarz, A., Uhlenbeck, K., Thom, R., Witten, E., and Zeeman, C. (1994). Responses to A. Jaffe and F. Quinn, "Theoretical mathematics: toward a cultural synthesis of mathematics and theoretical physics". *Bulletin of the American Mathematical Society*, 30(2):178–207.

Avigad, J. (2008). Computers in mathematical inquiry. In Mancosu, P., editor, *The Philosophy of Mathematical Practice*, chapter 11, pages 302–316. Oxford University Press, Oxford.

Bailey, D. H. and Borwein, J. M. (2005). Experimental mathematics: Examples, methods and implications. *Notices of the American Mathematical Society*, 52(5):502–514.

Bailey, D. H., Borwein, J. M., and Girgensohn, R. (1994). Experimental evaluation of Euler sums. *Experimental Mathematics*, 3(1):17–30.

Baker, A. (2007). Is there a problem of induction for mathematics? In Leng, M., Paseau, A., and Potter, M., editors, *Mathematical Knowledge*, pages 59–73. Oxford University Press, Oxford.

Baker, A. (2008). Experimental mathematics. *Erkenntnis*, 68(3):331–344.

Bassler, O. B. (2006). The surveyability of mathematical proof: A historical perspective. *Synthese*, 148:99–133.

Borwein, J. (2008). Implications of experimental mathematics for the philosophy of mathematics. In Gold, B. and Simons, R. A., editors, *Proof & Other Dilemmas: Mathematics and Philosophy*, chapter 2, pages 33–59. Mathematical Association of America, Washington DC.

Borwein, J. and Bailey, D. (2004). *Mathematics by Experiment: Plausible Reasoning in the 21st Century.* A K Peters, Natick MA.

Borwein, J. and Borwein, P. (1992). Strange series and high precision fraud. *The American Mathematical Monthly*, 99(7):622–640.

Borwein, J., Borwein, P., Girgensohn, R., and Parnes, S. (1996). Making sense of experimental mathematics. *The Mathematical Intelligencer*, 18(4):12–18.

Borwein, P., Erdélyi, T., and Littmann, F. (2008). Polynomials with coefficients from a finite set. *Transactions of the American Mathematical Society*, 360(10):5145–5154.

Borwein, P. and Jörgenson, L. (2001). Visible structures in number theory. *The American Mathematical Monthly*, 108(10):897–910.

Bown, W. (1991). New-wave mathematics. *New Scientist*, 1780:33.

Burkholder, L., editor (1992). *Philosophy and the Computer.* Westview Press, Boulder CO.

Ceruzzi, P. E. (2005). Moore's Law and technological determinism: Reflections on the history of technology. *Technology and Culture*, 46(3):584–593.

Chaitin, G. J. (1993). Randomness in arithmetic and the decline and fall of reductionism in pure mathematics. *Bulletin of the European Association for Theoretical Computer Science*, 50:314–328.

Corfield, D. (2003). *Towards a Philosophy of Real Mathematics.* Cambridge University Press, Cambridge.

Corry, L. (2008). Number crunching vs. number theory: Computers and FLT, from Kummer to SWAC (1850–1960), and beyond. *Archive for History of Exact Sciences*, 62:393–455.

Devlin, K. and Wilson, N. (1995). Six-year index of "Computers and mathematics". *Notices of the American Mathematical Society*, 42(2):248–254.

Echeverría, J. (1992). Observations, problems and conjectures in number theory — the history of the Prime Number Theorem. In Echeverría, J., Ibarra, A., and Mormann, T., editors, *The Space of Mathematics. Philosophical, Epistemological, and Historical Explorations*, pages 230–252. Walter de Gruyter, Berlin.

Echeverría, J. (1996). Empirical methods in mathematics. A case-study: Goldbach's Conjecture. In Munévar, G., editor, *Spanish Studies in the Philosophy of Science*, volume 186 of *Boston Studies in the Philosophy of Science*, pages 19–55. Kluwer Academic Publishers, Dordrecht.

Ekhad, S. B. and Zeilberger, D. (1996). The number of solutions of $X^2 = 0$ in triangular matrices over $GF(q)$. *Electronic Journal of Combinatorics*, 3(R2):1–2.

Epstein, D. and Levy, S. (1992). Message from the editors. *Experimental Mathematics*, 1(3).

Ferguson, H. R. P., Bailey, D. H., and Arno, S. (1999). Analysis of PSLQ: An integer relation finding algorithm. *Mathematics of Computation*, 68(225):351–369.

Franklin, L. (2005). Exploratory experiments. *Philosophy of Science*, 72:888–899.

Gallian, J. and Pearson, M. (2007). An interview with Doron Zeilberger. *MAA Focus*, 27:14–17.

Goldstein, C. (2008). How to generate mathematical experimentation, and does it provide mathematical knowledge? In Feest, U., Hon, G., Rheinberger, H.-J., Schickore, J., and Steinle, F., editors, *Generating Experimental Knowledge*, number 340 in MPIWG Preprints, pages 61–85. Max-Planck-Institut für Wissenschaftsgeschichte, Berlin.

Hales, T. C. (1994). The status of the Kepler Conjecture. *The Mathematical Intelligencer*, 16(3):47–58.

Horgan, J. (1993). The death of proof. *Scientific American*, 269(4):74–82.

Jaffe, A. and Quinn, F. (1993). “Theoretical Mathematics”: Toward a cultural synthesis of mathematics and theoretical physics. *Bulletin of the American Mathematical Society*, 29(1):1–13.

Jaffe, A. and Quinn, F. (1994). Response to comments on “Theoretical Mathematics”. *Bulletin of the American Mathematical Society*, 30(2):208–211.

Lakatos, I. (1976). *Proofs and Refutations: The Logic of Mathematical Discovery.* Cambridge University Press, Cambridge. Edited by John Worrall and Elie Zahar.

McEvoy, M. (2008). The epistemological status of computer-assisted proofs. *Philosophia Mathematica*, 16(3):374–387.

Medawar, P. (1979). *Advice to a Young Scientist.* Harper & Row, San Francisco CA.

Steinle, F. (1997). Entering new fields: Exploratory uses of experimentation. *Philosophy of Science*, 64(S1):S65–S74.

Steinle, F. (2002). Experiments in history and philosphy of science. *Perspectives on Science*, 10(4):408–432.

Thurston, W. P. (1994). On proof and progress in mathematics. *Bulletin of the American Mathematical Society*, 30(2):161–177.

Tymoczko, T. (1979). The four-color problem and its philosophical significance. *Journal of Philosophy*, 76(2):57–83.

Van Bendegem, J. P. (1998). What, if anything, is an experiment in mathematics? In Anapolitanos, D., Baltas, A., and Tsinorema, S., editors, *Philosophy and the Many Faces of Science*, chapter 14, pages 172–182. Rowan & Littlefield Publishes, Ltd., Lanham MD.

Van Kerkhove, B. (2005). Aspects of informal mathematics. In Sica, G., editor, *Essays on the Foundation of Mathematics and Logic*, pages 267–351. Polimetrica, Monza.

Van Kerkhove, B. and Van Bendegem, J. P. (2008). Pi on Earth, or mathematics in the real world. *Erkenntnis*, 68(3):421–435.

Wilson, R. (2002). *Four Colours Suffice. How the Map Problem was Solved.* Penguin/Allen Lane, London.

Zeilberger, D. (1993). Identities in search of identity. *Theoretical Computer Science*, 117:23–38.

Zeilberger, D. (1994). Theorems for a price: Tomorrow's semi-rigorous mathematical culture. *The Mathematical Intelligencer*, 16(4):11–14, 76.