Computational Paths to Discovery with Optimization

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VISION

In the future it is conceivable that computers will take an active role in the creative process of doing mathematics. Routine parts of proofs will more and more be performed by computers. Already ten years ago the British mathematician Timothy Gowers (Cambridge University) speculated: "I expect computers to be better than humans at proving theorems in 2099". Gowers is one of the most brilliant and influential mathematicians of our days: In 1998 he got the Fields medal, which is the mathematical equivalent of the "Nobel prize". He is the editor of *The Princeton Companion to Mathematics*. Furthermore, he is a very active user of the Internet and we highly recommend to look at his blog, the "polymath project", and the "tricki web site".

So, what happened during the last ten years? Are we — humans and computers — coming closer to Gowers' speculation? In this article we would like to illustrate that already now computers are *sometimes* better than humans at proving theorems, and that doing computer-assisted mathematics is fruitful, useful and most important: It is fun.

PARADIGM

In the last years we attacked several problems in geometry and optimization with a symbiosis of human and computer reasoning. One of our motivations is that we want to find systematic ways for doing elegant and insightful computer-assisted proofs. Typically one works with the following three-step process:

1. Modelling

Modelling the problem (or a relaxation of it) as an optimization problem is usually very beneficial, because there is a wealth of theoretical and practical methods. For an efficient treatment, a better understanding of the structure of the space of all possible solutions (e.g. its symmetry, its regularity) is usually needed. This step is often difficult, but once achieved, this can lead to new insights.

2. Solving

Solving a problem computationally usually involves the design of new optimization techniques on top of existing standard procedures. Here it is important to separate algebraic and numerical calculations to find a good balance between accuracy and speed of computation.

3. Interpretation

Obtained numerical results have to be turned into rigorous mathematical arguments. "Beautification" of numerical data often leads to the discovery of new objects or previously unrevealed structure of the problem.

As examples for this three-step process, we describe some of our recent work. Other fascinating examples are for instance in [3].

KISSING NUMBER

In geometry, the *kissing number* is the maximum number of non-overlapping equally-sized spheres that can simultaneously touch a central sphere. The kissing number is only known for dimensions 1, 2, 3, 4, 8 and 24. It is easy to see that the kissing number in dimension 1 is 2, and in dimension 2 it is 6. The kissing number problem has a rich history. In 1694 Isaac Newton and David Gregory had a famous discussion about the kissing number in three dimensions. The story is that Gregory thought thirteen spheres could fit while Newton believed the limit was twelve. Only in 1953, Schütte and van der Waerden proved Newton right.

In the 1970s advanced methods to determine upper bounds for the kissing number based on optimization, namely linear programming, were introduced. Using these new techniques, the kissing number problem in dimension 8 and 24 was solved. For four dimensions, however, the optimization bound is 25, while the exact kissing number is 24. In a celebrated work Oleg Musin (University of Texas at Brownsville) proved this in 2003, see [8].

Figure 1: *Construction of 12 kissing spheres. Image credit: Anja Traffas*

In collaboration with Christine Bachoc (Université Bordeaux) we found new upper bounds for kissing numbers. There we gave a unified proof of all known kissing numbers and we found new upper bounds in all other dimensions up to 24 with numerical assistance of Hans Mittelmann (Arizona State University).

In [1] and [7] we found a rigorous, computational proof for these new upper bounds. The first two phases of the three-step process were especially important: In step 1 we used semidefinite programming which is more powerful than linear programming and we used Fourier analysis for exploiting the rotational symmetry of the problem. In step 2 we applied techniques from polynomial optimization which were introduced by Jean Lasserre (Université Toulouse) and Pablo Parrilo (MIT) only recently. These algebraic methods enabled us to give a rigorous mathematical proof.

ENERGY MINIMIZATION

The kissing number problem is not only a nice geometric puzzle problem, but it is related to many problems in science and technology. It belongs to a class of more general energy minimization problems. Given some potential function f, defined on pairs of points, how should points on a sphere be arranged to minimize the total f-potential energy? For a configuration C of points on the unit sphere, this f-potential energy is defined by

$$E_f(C) = \sum_{x,y \in C, x \neq y} f(x,y).$$

Popular choices of potential functions are

$$f(x,y) = \frac{1}{\|x-y\|^s} \tag{1}$$

with a fixed parameter $s > 0$. For $s = 1$ and in dimension 3 one obtains for example the Coulomb potential studied in physics. A typical question is to find a configuration of N points on the unit sphere which minimizes the f-potential energy among all configuration with N points. By letting s tend to infinity one can see that the kissing number problem is a limit case of energy minimization. Another

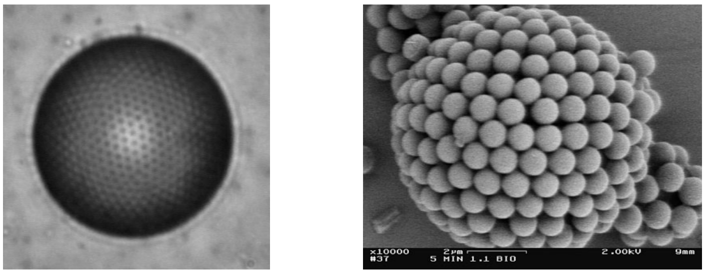

Figure 2: *Microscope images of "colloidosomes", water droplets coated by polystyrene beads, all submerged within an oil emulsion. Image credit: David Weitz research laboratory, Experimental Soft Condensed Matter Group at Harvard University* `http://www.deas.harvard.edu/projects/weitzlab/`

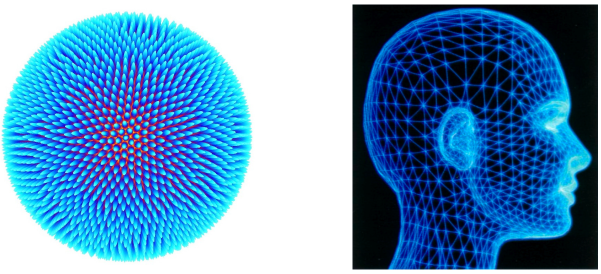

Figure 3: *Image credit: Left: Rob Womersley, "Interpolation and Cubature on the Sphere",* `http://web.maths.unsw.edu.au/~rsw/Sphere/`
Right: Laurent Orluc, "Pointillisme", `http://www.math.vanderbilt.edu/~esaff/pointillisme.html`

way to model the kissing number problem as an energy minimization problem is by using the potential function

$$f(x, y) = \begin{cases} \infty, & \text{if } \|x - y\| < 1, \\ 0, & \text{otherwise.} \end{cases}$$

Then the kissing number is the maximum number N so that there is a point configuration with N points on the unit sphere with finite f-potential energy. In this case the point configuration gives the touching points of the spheres.

Energy minimizing point configurations on spheres have attracted mathematicians in fields such as approximation and coding theory, and biologists, chemists, and physicists in diverse fields such as viral morphology, crystallography, molecular structure and electrostatics. As engineers advance in gaining control of the microscopic and even nanoscopic world, energy minimization principles appear to become increasingly important for synthetic fabrication and design. Figure 2 for example shows two microscopic images of tiny polystyrene beads (one of the most widely used kinds of plastic), on the surface of water droplets. These "colloidosomes" are self-assembling according to energy minimizing principles and are expected to be of future use in medical applications such as drug delivery.

The distribution of particles on more general surfaces and manifolds has applications in a variety of fields where discretization is needed, such as interpolation or computer aided design (see Figure 3 and [6]). The distribution of particles in Euclidean space has been of particular interest. As in the case of spherical point configurations, where the limit case is the kissing number problem, there is a well known problem giving the limit case of energy minimization: the sphere packing problem. It asks for the densest possible arrangement of non-overlapping, equally sized spheres. Its three-dimensional version became known as "Kepler conjecture". After a long and controversy history, it has in recent years been solved with massive computer calculations by Thomas Hales (University of Pittsburgh). Here step 2 of the paradigm was the most difficult part.

Finding energy minimizing point configurations on spheres and in Euclidean space is often done with computer simulations. With the right model at hand, and by assuming some prescribed structure (step 1), such computer experiments can lead to the discovery of new geometric structures. Together with Henry Cohn (Microsoft Research) and Abhinav Kumar (MIT) we have found in [2] and [4] several previously unknown point configurations on spheres and in Euclidean space. Some of them are conjectured to be "universally optimal"; meaning they minimize energy for a large class of potentials, including all those defined by (1). These amazing configurations would most likely not have been discovered without computer assistance. The newly found energy minimizing point configurations in Euclidean space, suggest a deeper, not yet understood symmetry of the Gaussian core model, which is one of the most interesting soft-core potentials studied in physics. These works exemplary show how in step 3 of the paradigm, computers may help to discover mathematical structure that was previously unknown.

GETTING CLOSER TO THE VISION

Where do we stand now? Nine decades before 2099? As described above, for certain classes of optimization problems, computers are already today an indispensable tool. Computers are also already better in checking the correctness of proofs. Proofs for theorems like the Jordan curve theorem or the four-color theorem can be checked by computers nowadays. The "FlysPecK" project of Thomas Hales [5] seeks to formalize his proof of the Kepler Conjecture in the computer theorem prover `HOL Light` which is based on the ML programming language.

Finally: There is a myth about Barbarossa, a German emperor who died during the Third Crusade. A legend grew that he was still alive, asleep in a cave. He would awake only when Germany needed him. In the 1930's somebody asked David Hilbert, "If you were to be awoken like Barbarossa, after five hundred years of sleep, what would you do?" Hilbert replied: "I would ask: Has anyone proved the Riemann Hypothesis?" Nowadays he would add: "Was it a human or a computer?"

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