A Balancing Act with Numerics and Computer-Aided Proofs (the case study of Equilibrium Measures)

A. Research context

Computer-aided mathematics have been developed in the last 20 years [14, 7, 8], and this trend is getting more and more important. Check for instance [3, 2], take a look at the increasing number of workshops which reunite computer scientists and well-known mathematicians [1][2] in an accelerated effort of theorem formalization or even listen to podcasts where one wonders whether AI will become a mathematician[3].

In this setting, computational mathematics (and in particular numerical methods) may play an underrated role as they have traditionally been used "only for experiments" and not as proofs. Of course, the vast majority of today's computer computation in science and engineering relies on the good old floating-point numbers and its inherent tedious proofs of last correct digit or more properly said –output accuracy of a numerical algorithm–.

In an attempt to bridge the gap between *experimental mathematics* and *computer proofs*, the field of *rigorous computing* (sometimes called *validated computing* as well) uses numerical computations, yet is able to provide rigorous mathematical statements about the obtained result, such as sure and reasonably tight, error bounds. Traditional validated computing [15] methods are based on arbitrary precision libraries and interval arithmetic computations [10], a simple set arithmetic, which always returns an interval guaranteed to contain the correct result. However, for most proofs involving current numerical methods, it is not enough just to juxtapose computer science and mathematics, but one needs to closely combine several branches of these two disciplines in order to design algorithms that calculate precisely (approximation theory, numerical analysis), efficiently (study of algorithms' complexity) and rigorously (computer algebra, validation methods, formal proofs).

Examples of computations with guaranteed numerical accuracy are present for instance in theoretical proofs in dynamical systems [14, 5], specific implementations of special functions for mathematical libraries [11] or more practical engineering problems like the control of spacecraft engines or orbital collision risk mitigation [13].

We focus on symbolic-numeric methods for obtaining validated algorithms. We are interested in improving their theoretical computational complexity as well as practical computer arithmetic aspects. More precisely, modern computer algebra algorithms (rooted in commutative and differential algebra) are employed via approximation theory (in suitable functional spaces) to obtain efficient approximations and analytic error bounds. Furthermore, at subsequent numerical levels, computer arithmetic problems are dealt with, especially in the context of roundoff errors or extended precision. Note that we aim not only to compute *approximations*, but also *enclosures* of errors.

B. Internship subject

Validated computing tools have already been used for several "classical" problems in real analysis (e.g., solving differential equations, numerical integration). They have been, however, considerbaly less developed and used in measure-theoretic frameworks for optimization. As a starting point in this direction, we propose to focus on a "much simplified" problem, which connects: (1) more mature validated algorithms for the evaluation of special functions which are solutions of certain differential equations in the complex plane and (2) an optimization problem on the space of Borel probability measures.

More specifically, the goal of the internship is to develop tools and algorithms for validated computations of equilibrium measures for logarithmic potentials, which essentially model the distribution of

[1] https://www.ipam.ucla.edu/programs/workshops/machine-assisted-proofs/
[2] https://aimath.org/workshops/upcoming/compproofs/
[3] https://www.quantamagazine.org/can-computers-be-mathematicians-20220629/

charges on a conductor under the influence of an external field. They have many applications ranging from the distribution of eigenvalues of large random matrices to the zeros of orthogonal polynomials with respect to exponential weights. Very efficient numerical techniques have been recently developed in literature [12, 6] and we aim at exploring several possible adaptations to the validated setting. We start with a toy model, of a known one dimensional real analytic external field $V : \mathbb{R} \to \mathbb{R}$, which has sufficient growth at infinity, with $\frac{V(x)}{\log|x|} \to \infty$ as $|x| \to \infty$. The question is to find the unique probability Borel measure $\mathrm{d}\mu(y) = \psi(y)\mathrm{d}y$ which minimizes:

$$\int\int \log\frac{1}{|x-y|}\mathrm{d}\mu(x)\mathrm{d}\mu(y) + \int V(y)\mathrm{d}\mu(y).$$

It is well known [4] that in this case the (essential) support of the equilibrium measure supp μ consists of a finite number of intervals. In particular when V is a polynomial of degree $2m$ the number of intervals is at most $2m+1$. This problem can be very efficiently numerically solved [12]. By this we mean that numerical approximations of both the support and the density ψ of the measure can be obtained with arbitrary precision. In particular, the density ψ is approximated using a truncated series, once the support is numerically found.

Several questions are left to be investigated:

- Can one provide a constructive *a posteriori* proof that the obtained numerical approximation is *ε-close* to the true mathematical equilibrium measure and provide an explicit bound for the numerical error?

  Note that in the case of a strictly convex V, the support of the optimal measure is a unique interval and the method of [12] allows for constructing a Newton operator which converges towards a unique root. This would imply a simplified, yet not completely trivial procedure for the error enclosure. One may make use of so-called rigorous Chebyshev approximations which were developed in [9].

- When the support consists of a union of intervals, a Newton operator adapted for this case converges towards the true equilibrium measure whenever the initial guess is sufficiently accurate. Thus, it is not possible to guarantee an *a priori* convergence. An *a posteriori* verification was proposed in [12] following an adaptation of the strong Euler–Lagrange variational conditions: there exists some constant $\ell \in \mathbb{R}$ such that

$$\begin{aligned} 2\int \log\frac{1}{|x-y|}\mathrm{d}\mu(x) + V(y) &= \ell, && \text{for } y \in \operatorname{supp}\mu \\ 2\int \log\frac{1}{|x-y|}\mathrm{d}\mu(x) + V(y) &\geq \ell, && \text{for all } y \in \mathbb{R}. \end{aligned}$$

  An adaptation of the method of [12] using interval arithmetic seems possible. Currently, in order to find the number of intervals in the support, the *a posteriori* validation procedure is used iteratively by testing with one, two – and so on– intervals. It would be interesting to further analyze the convergence of the Newton operator and establish further unicity conditions without proceeding iteratively.

- Finally, if the time permits, one could extend this study to analyze the link with other related moment-constrained problems, especially those treated in [1] using a computer algebra approach.

C. Internship location

This internship is supervised by Mioara Joldes[4] at LAAS-CNRS in Toulouse. Further collaborations with S. Olver at Imperial College London as well as a related subject for a PhD thesis are possible.

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