Studying PDE dynamics via optimization with integral inequality constraints

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1 Recent Developments and Open Problems

A sizeable fraction of the discussion during the FRG centered on the pointwise dual relaxation (PDR) method described in [1, 3] and references therein. This is a method for relaxing integral variational problems into sum-of-squares (SOS) polynomial optimization problems. In general it is an open problem to characterize when this method introduces a relaxation gap and so cannot converge to the global optimum of the original integral variational problem. Partial results that guarantee sharpness under fairly strong assumptions, and that give counterexamples to sharpness in other cases, have appeared this year in preprints by FRG participants [2, 4]. As for computational implementation of this relaxation strategy for particular variational problems, the examples published so far [1, 3] are simple enough that they could have been solved by more standard computational strategies. It has remained a practical challenge to produce computational results using the PDR method for examples that are intractable by existing methods. **[David: What about various examples in Valmorbida et al's work? There are some PDE dynamics problems that maybe are hard to solve otherwise.]**

2 Scientific Progress Made

Parts of each day were devoted to informal presentations from various participants on recent progress. Fantuzzi and Tobasco presented their results [2] on sharpness conditions for the PDR method, and Korda presented his results [4] on the same topic. The results are complementary with neither being contained in the other. Korda's coauthor joined some conversations via zoom, and the discussions led to an updated version of their main counterexample, reflected in the third version of [4] on the arXiv. Tobasco presented topics from variational analysis, including quasiconvexity and polyconvexity, and possible applications of SOS optimization were explored. Examples include verifying that a function is or is not quasiconvex, or constructing the largest possible supporting functions that are polyconvex.

Fantuzzi and Fuentes shared unpublished work on a computational approach to integral variational problems that is a possible alternative or complement to the PDR approach. Their method relies on finite element discretizations of the variational problem and SOS computations for the discretized problems. Under reasonable assumptions this is guaranteed to converge to the optimum of the original problem with increasing finite element resolution and polynomial degree, and it even provides global optimizers to the discretized problems. Computational cost makes it hard to reach convergence for 2D problems, and, unlike the PDR method as polynomial degrees are raised, the convergence is not monotone. Nonetheless, some promising computational examples were shown, and an effort was begun to compute results for the same examples using the PDR method so that a one-to-one comparison can be made.

3 Outcome of the Meeting

Collaborations were initiated on many different projects and involving many different subsets of participants. Here we describe only a few representative topics.

3.1 Questions concerning the combination of finite elements and SOS

Fantuzzi and Fuentes studied integral variational problems problems of the form

$$f^* := \min_{u \in W_0^{1,p}(\Omega)} \int_\Omega f(x,u,Du)\,\mathrm{d}x, \tag{1}$$

where $\Omega \subset \mathbb{R}^n$ is a Lipschitz domain, $f : \Omega \times \mathbb{R}^m \times \mathbb{R}^{m\times n}$ is a quasiconvex polynomial function, and $W_0^{1,p}(\Omega)$ is the usual Sobolev space of weakly differentiable p-integrable functions vanishing on the domain boundary. Their approach approximates optimal u using a “discretize & relax” approach consisting of two steps. First, the variational problem is discretized on a finite element mesh whose elements have size h. This transforms problem (1) into a polynomial optimization problem (POP) where the number of variables is inversely proportional to h, but which has a high degree of structure. Specifically, variables are coupled directly only if they are used to represent the function u on a single mesh element. The second step is to use sum-of-squares polynomials of degree $\omega \in \mathbb{N}$ to relax this POP into a convex semidefinite program (SDP), whose optimal value $\lambda(\omega,h)$ bounds that of the POP from below. Under suitable technical conditions, one can show that

$$\lim_{h\to 0} \lim_{\omega\to\infty} \lambda(\omega,h) = f^*. \tag{2}$$

Moreover, the solutions of the SDP relaxations converge to the optimal u when the latter is unique.

Despite these initial results, more should be done to better understand the theoretical properties of this approach and, consequently, make it more useful in practice. This FRG identified three areas where progress is desirable.

Order of limits Can the order of limits in (2) can be reversed? If so, what is the $h \to 0$ limit of the SDPs obtained with fixed relaxation order ω? Such questions are not just a mathematical curiosity: a full understanding of the $h \to 0$ limit for fixed ω could lead to a new type of convex relaxations for (1) which, contrary to existing convexification approaches, produce arbitrarily accurate lower bound on the global minimum f^*. Some progress was made by considering the setup of periodic domains and optimizing over periodic functions, which leads to an optimization over polynomials with infinitely many variables, but the lack of a positivity representation theorem of such mathematical objects, even for a compact domain, is an obstacle.

Removing technical assumptions The known proof of (2) requires two restrictive technical assumptions. The first is the so-called *running intersection property* (RIP), which requires the coupling between variables of each finite-element discretization to be described by a chordal graph. This condition is never satisfied for variational problems over two- or higher-dimensional domains Ω, unless one introduces “fictitious” variable couplings that increase computational costs to prohibitive levels. On the other hand, practical experience suggests that the RIP may often be unnecessary. This FRG discussed the possibility of dropping the RIP requirement by exploiting a connection with the PDR method. Specifically, some of the participants sketched an argument showing that the RIP is unnecessary if the PDR method is sharp. What remains to be done is to rigorously confirm this and to prove more the sharpness of the PDR method for more interesting classes of problems than those studied by the participants in [2] and [4].

Further discussion revolved around a second restrictive technical assumption required to prove (2): the uniqueness of the (global) minimizer of (1). In general, the optimal solutions of the SDP relaxations converges to the sequence of moments of a probability measure supported on the set of global minimizers of (1). If multiple minimizers exist, individual ones can be recovered only if the SDP relaxation for a given finite ω and h is exact (meaning that it gives a sharp bound on the finite-element discretization for mesh size h) and its matrix variables satisfy a rank condition called “flatness”. These finite convergence and flatness conditions often hold in practice, but there is currently no proof that they hold generically for SDP relaxations that exploit the POP structure. (They do when the structure is ignored, but this is clearly not desirable in practice.) An alternative to bypass this problem would be to find extreme optimal solutions to the SDP relaxations, which are moment sequences of probability measures supported on individual minimizers. To the best of our knowledge, however, no SDP solvers have the ability to reliably produce extreme solutions.

Efficient solution of large-scale SDP relaxations In addition to theoretical questions, the “discretize & relax” of Fantuzzi & Fuentes poses practical challenges. Indeed, the SDP relaxations one must solve for small mesh size h and/or large relaxation order ω are beyond the reach of available general-purpose SDP solvers. This is especially true when tackling integral variational problems in two or more spatial dimensions. One possible way forward is to exploit the particular structure of the SDP relaxations. It seems possible to combine a variation of recently developed decomposition strategies for SDPs with “first-order” algorithms, such that each iteration of the algorithm consists of many small independent subproblems that can be solved efficiently and—crucially—in a distributed manner. While the formulation of such algorithms is relatively straightforward, there are many possible variations and it is unclear which one will offer the best compromise between iteration simplicity, parallelization, and speed of convergence. Answering this question will require efficient software prototypes as well as further theoretical convergence analysis.

3.2 Application areas for the PDR method

An application area that lies outside existing sharpness guarantees for the PDR, but where improvement on existing analytical results seems possible, is the estimation of optimal constants for a linear Korn’s inequality, which allows one to control the full gradient of a map $u : \Omega \subset \mathbb{R}^d \to \mathbb{R}^d$ in terms of its symmetric gradient. We work in dimensions $d \geq 2$ and define $e_{ij}(u) = \partial_i u_j + \partial_j u_i$ for $i, j = 1, \ldots, d$. Without boundary conditions, the inequality guarantees the existence of C such that

$$C \int_\Omega |e(u)|^2 \geq \min_{W \in \mathrm{Skew}} \int_\Omega |\nabla u - W|^2$$

for all $u(x)$. With periodic boundary conditions, that

$$C \int_{\mathbb{T}^d} |e(u)|^2 \geq \int_{\mathbb{T}^d} |\nabla u|^2$$

for periodic $u : \mathbb{T}^d \to \mathbb{R}^d$. These are classical inequalities in the theory of elasticity, but the optimal constants C are unknown except in very simple domains. We wish to compute convergent approximations to the optimal constants, and to find the $u(x)$ that saturate these optimal constants. The PDR method is directly applicable in the case without boundary conditions, and ways to implement periodic boundary conditions were discussed.

A second application concerns the question of how much energy is required to carry out elastic crumpling. We seek sharp lower bounds on a model problem:

$$\min_{(u,w):\mathbb{T}^2 \to \mathbb{R}^2 \times \mathbb{R}} \int_{\mathbb{T}^2} |e(u) + \frac{1}{2}\nabla w \otimes \nabla w - I|^2 + h^2 |\nabla\nabla w|^2 \, dx.$$

Letting $E_h(u,w)$ denote the above energy functional, the minimum is known to obey $\min E_h \lesssim h^{5/3}$ by a “minimal-ridge” construction that suitably smooths an origami crease pattern. It is also not hard to prove that $\min E_h \gtrsim h^2$, and a more subtle argument shows the better asymptotic bound $\min E_h \gg h^2$. It is widely believed that the upper bound is sharp, meaning there are positive constants C and C' such that

$$Ch^{5/3} \leq \min E_h \leq C' h^{5/3}$$

for $h \leq 1$. Thus we aim to apply the PDR method to find a lower bound strictly better than $E_h \gg h^2$, and perhaps scaling like $h^{5/3}$.

References

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