PhD-position: Non-convex optimization with applications in imaging.

Overview

Imaging is a mathematical field which consists of using indirect measurements (data) for reconstructing (images of) structures which can not be seen directly. This appears for example in mathematical tomography, where the interior of objects (such as a human being) can be reconstructed by X-ray absorption patterns. When imaging on an atomic level, one retrieves e.g. crystal structures from the amplitude of diffraction patterns, using highly monochromatic light. The problem of algorithmically converting the data to the desired image is known as phase retrieval. Such methods will be important for e.g. the beamline NanoMax at MAX IV, Lund, as well as ESS later on. When formulated in mathematical terms, these problems belong to the class of “ill-posed inverse problems”, which usually are solved by optimization tools upon adding additional constraints (related to prior knowledge) to stabilize the inversion process. This boils down to finding the minimum of certain functionals which usually are non-convex, which has the effect that most algorithms are ad-hoc with no guarantees of convergence and/or lacks concrete characterizations of the point of convergence. For this reason it has become very popular to replace the desired functional with a “similar” one which is convex. This has the advantage of yielding algorithms which are guaranteed to converge, but the disadvantage that the optimal point is not the one initially sought, and it is well known that these methods always give rise to biased solutions.

Recently, our team has made advances in this direction [17]. The paper is the culmen of several years of research devoted at understanding convergence of algorithms in non-convex settings, and of computing convex envelopes of non-convex functionals [3, 10, 11, 14], thereby being able to provide convergence proofs of related algorithms as well as descriptions of the convergence points. We have also developed several algorithms for tomographic reconstructions [8, 9] which triggered a close collaboration with the MAX IV laboratory imaging group. The PhD student (Viktor Nikitin) who developed these algorithms and defended his thesis at the Mathematics department in 2016, is currently implementing the new algorithms at the MAX IV Laboratory and LUNARC as a PostDoc hosted at the MAX IV Laboratory. The open PhD-position is intended to further strengthen the link between the Centre for Mathematical Sciences and MAX IV. We aim to continue the study of the above mentioned areas (non-convex optimization, fast algorithms) with a particular focus on their potential use for MAX IV and their future users, as well as the National 7T facility (MRI) and later on ESS (neutron tomography). MAX IV is currently the most intense light-source on the planet, and due to new technology also the most monochromatic beam. However, this will have a limited impact unless coupled with new imaging algorithms and on-site expertise who can guide the users on how to extract the desired information from the acquired data. As mentioned, the phase retrieval problem, which appears in coherent diffraction tomography and ptychography, is of particular interest for the beamline NanoMax and can be used for the imaging of e.g. crystals and particles. A related problem which we wish to tackle is that of inverting measurements of an object which is deforming during the tomographic acquisition. A typical example is clinical observations of moving organs or the emerging field of micrometer resolution functional anatomy of small animals [29]. As of today only indirect methods are used to measure the function of the lung tissue. Yet to understand the underlying mechanism of lung malfunctions the microstructure of the organ must be studied in vivo. So far the only promising way is using synchrotron X-ray tomographic microscopy, but the problem of reconstruction of the moving organ at the micrometer scale is not solved. Incidentally, the same type of problem is of interest to the Cardiac MR group at the National 7T facility at LBIC/Slåtens Universitetssjukhus, for example when doing MRI-imaging on the heart [25], and they are also interested in collaboration on this matter. In our group we have worked with a lot of different problems during the last couple of years. We have published work in complex analysis and operator theory [2, 4, 12, 16, 18], inverse problems [1, 3], fast algorithms [8], optimization [17, 3, 10, 11, 14], geophysics [5] and signal processing [6, 7, 13]. Our aim is to be active on the entire chain of problems, ranging for pure mathematical analysis to the development of fast numerical algorithms.
to the actual treatment of measured data. Despite the applied flavor of the project, the mathematical problems to be tackled are by no means easy or only in the area “applied mathematics”. The position is suitable for a person who likes pure mathematics but at the same time has knowledge and interest in developing and numerically testing algorithms. Below we list in greater detail some different components of the planned research.

**Inverse problems/non-convex optimization**

In many physical and engineering setups one seeks information about a physical object or system that can only be measured indirectly. The problem of reconstructing the information of interest is called an inverse problem, and these are usually ill-posed. This means that additional assumptions need to be added in order to obtain stable reconstruction algorithms. A lot of attention has recently been put in replacing traditional constraints on amplitude or frequency range by imposing various types of sparseness constraints on the solutions. A good motivation for this concerning imaging technologies is that most images can typically be substantially compressed without losing much information content. Imposing such conditions will, however, cause the inverse problem to become non-linear even if the original formulation is linear. Related optimization problems are then non-convex and these are difficult to deal with due to the presence of local minima. For this reason, it is important to try to find formulations that lead to convex or close to convex optimization problems. There is an abundance of algorithms using optimization methods of various kinds that attempt to solve non-convex/non-linear inverse problems with various degrees of success. Many of them are ad-hoc type of algorithms, where the “solution” obtained is merely the output of some algorithm without actually solving a well defined problem, since they often get stuck at a local minimum. This also hold for inverse problems that are non-linear already in their original formulation, such as the phase retrieval problem and the complex frequency estimation problem.

An interesting approach that can be taken to address these issues relies on replacing the original non-convex objective function with its convex envelope. It has recently turned out that there are important cases where it is possible to compute the convex envelope explicitly [27, 17, 3, 11, 14], or one may work with it implicitly in the problem formulation to prove convergence of seemingly ad-hoc methods [10].

When looking for sparse solutions one is interested in minimizing the amount of non-zero contributions, sometimes called the $\ell^0$-penalty. This is however non-convex, even discontinuous, and a popular alternative is to add an $\ell^1$-penalty on the data terms (as in e.g. compressed sensing). This has the advantage that it leads to a convex functional, and under some conditions the solutions coincide with those of the first (non-convex) problem [15, 21, 36]. However, the region where this happens is quite limited, and many physical setups work in regimes where this is not the case. One problem is for instance that the $\ell^1$-penalty will enforce a bias on the obtained solution, where the amplitudes are consequently underestimated.

Attempts to solve these problems typically fall into three categories, either one change the problem formulation (and its solution) by replacing the actual cost-functional with a standard convex one ($\ell^1$-minimization, nuclear norm, compressed sensing etc.), or one builds ad hoc semi-convex functionals using e.g. $\ell^p$-norms with $0 < p < 1$ and demonstrate that these “seem to do well in practice”, or one leaves the non-convex functional as is and rely on classical algorithms which often get stuck in local minima or even diverge occasionally (like alternating projections, Douglas-Rachford, ADMM and so on), often combined with restart schemes. We wish to provide a 4th alternative by continuing the investigation mentioned above.

The original motivation for using the nuclear norm was given by [22] where it is shown that the nuclear norm is the convex envelope of the rank function on the set $\{A; \|A\| \leq 1\}$. The constraint $\|A\| \leq 1$ is artificial and added since the convex envelope on the whole domain would simply be the zero function. Recently it has been observed [27, 28] that this problem can be circumvented if one takes into account the least squares penalty term $\|A - F\|^2$ before taking the convex envelope. The replacement of the rank penalty arising in this way is non-convex by itself (but convex when combined with $\|A - F\|^2$) and has the property of being equal to the original non-convex one far away from discontinuities, leading to global minima which often even coincide with the originally sought one. In contrast, the nuclear norm always move the sought optimum because it penalizes large and small singular values alike and therefore exhibit a shrinking bias. We have recently shown that the basic idea behind [27, 28] is very general and does not restrict itself to low rank approximation. Consider a non-convex problem of the form

$$\arg\min_{X \in \mathcal{M}} f(X) + \|Z(X) - F\|^2.$$  \hspace{1cm} (0.1)
over some subset \( \mathcal{M} \) of a Hilbert space \( \mathcal{H} \), (where previously \( X \) was a matrix, \( f(X) \) its rank, \( \mathcal{L} = \text{Id} \) and \( F \) measured data). In other words we are seeking the value of \( X \in \mathcal{M} \) for which the minimum is attained. It turns out that when \( \mathcal{L} = \text{Id} \) the convex envelope of this functional also is of the form \( \hat{f}(X) + \|X - F\|^2 \) where \( \hat{f} \) is the so called Lasry-Lions approximant (previously used in regularization) which can be explicitly computed in a number of concrete situations \([17]\). Replacing the original functional by this leads to a convex problem which is much closer to the original problem than previously considered alternatives in the literature. Related algorithms can be proven to converge and their output can be analyzed by understanding the minimal points of \( \hat{f}(X) + \|X - F\|^2 \) on \( \mathcal{M} \). When \( \mathcal{L} \neq \text{Id} \) it is still possible to prove that the replacement of \( f \) by \( \hat{f} \) has a number of desirable features, such as not moving global minima (although convexity might be lost) \([17, 3]\). Recently we have also been able to give criteria of when sparse stationary points to such functionals are actually unique, i.e. when the point of convergence actually solves the original problem despite lack of convexity \([33]\). A partial aim of the PhD work is to further develop these ideas and also apply them to synchrotron tomography, MRI and seismic imaging.

**Phase retrieval**

Given a complex signal \( F(k) \) with phase \( \psi(k) \), i.e. \( F(k) = |F(k)|e^{i\psi(k)} \) the “phase retrieval problem” consists in finding \( \psi \) given measurements only of the amplitude \( |F(k)| \) and a set of constraints. Phase retrieval problems in two or three dimensions arise for both near field imaging (real space imaging described by the Fresnel transform) \([19]\) and far field (coherent diffraction) imaging \([23]\). In the early 1980’s \([23, 24]\), it was demonstrated that if the diffracting sample has a small support and if the diffraction patterns is adequately measured, it is possible to retrieve the phase using an iterative approach now known as the Gerchberg-Saxton-Fienup-algorithm.

Since the first experimental demonstration realized in 1999 by Miao et al. \([31]\) using a synchrotron X-ray beam, coherent diffraction imaging (CDI) has significantly progressed and been applied to the reconstruction of shape but also strain inside nanocrystals \([34, 35]\). Many efforts have also been made to improve the ab. initio phase retrieval algorithms, combining the original iterative algorithm (Gerchberg-Saxton-Fienup) with charge flipping algorithms \([38]\), and more recently using ptychography \([20]\). Another direction is the shrink wrap algorithm, in which the support of the object is a constraint which is iteratively updated to fit the measurements \([30]\). The paper \([32]\) from 2010 gives an overview of contemporary algorithms for phase retrieval and concludes with (p. 65) “It must be observed, however, that none of these approaches have yielded an algorithm that has been found to converge in all cases.” This continues to be the case, as indicated by the recent publication \([26]\) which provides state of the art algorithms for the solution of both ptychography and traditional phase retrieval.

In collaboration with Gerardina Carbone (NanoMax) and Jesper Wallentin (Synchrotron Radiation Research, LU) we plan to work on improvements of these algorithms, based on the new ideas emerging from the previous section.

**4D-imaging**

In transmission tomography as well as MRI-measurements on humans, a problem is blurring due to the fact that the object measured is not still during the measurement process (see e.g. \([25, 37]\)). Popular methods for dealing with this problem involve optimizaioon techniques of the type discussed above. For example, in \([25]\] the total variation norm is used in both spacial variables and time, to stabilize the inversion process. However, the scientists with a need for such methods are usually not mathematicians (some are doctors) and do not have the time to improve or tailormake these algorithms. For example, the lungs move in a continuous fashion when healthy whereas undergoes unpredictable distortion during an asthma attack. Such differences affect the design of the corresponding algorithm. Consequently, much data acquired at synchrotron imaging beamlines or the National 7T facility (at LBIC/Skånes Universitetssjukhus) is sub-optimally processed, or in worst cases not processed at all mainly because the ambitious acquisition schemes do not match the current capabilities of the reconstruction methods. In collaboration with Rajmund Mokso (MedMax) and the cardiac imaging group at the National 7T facility, we plan to work on improvements of such algorithms.
References


