A research agenda for iterative approaches to inverse problems using evolutionary computation

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***Abstract*—**
This position paper addresses the relevance of evolutionary computation for iterative approaches to inverse problems. We focus on a set of six real-world problems selected from the areas of space dynamics, materials science, geophysics, heat transfer, oceanography and meteorology. These problems are far from being trivial and their associated direct models yield a wide structural diversity, thus providing a rich sample of the space of inverse problems. We neither discuss any particular problem in depth, nor present any results obtained so far. Our emphasis is on the research agenda defined by them, for the issue of deriving a generic methodology for approaching inverse problems that has evolutionary computation in its core.

I. Inverse Problems

An inverse problem (IP) is to determine

> "unknown causes based on observation of their effects. This is in contrast to the corresponding direct problem, whose solution involves finding effects based on a complete description of their causes"

(citation in [22] attributed to Alifanov, a pioneer of inverse methods). For a rigorous definition see [17]. Inverse problems are mathematically ill-posed in the sense that the existence, uniqueness and stability of solutions cannot be assured.

As an example, consider the situation in which there is an electromagnetic signal being transmitted by a source on the surface of the Earth, and there is a satellite in orbit such that it can be reached by the signal. A direct problem in this case would be: given the position of the source, the position and velocity of the satellite at a given moment, the transmission frequency of the source, and a few other features that fully characterise the situation, find out the Doppler shift of the source's transmission frequency, as perceived by the satellite. In contrast, given the Doppler shift (together with the various other features mentioned above), the IP in this case could be finding out the position of the source.

IPs are ubiquitous in many areas of science and engineering, such as meteorology, heat transfer, electromagnetism, material science, etc. In remote sensing, for instance, this is a recurring fact due to the necessity of having to infer vertical profiles (above or below the surface of Earth) from remotely collected data of the surface. The ability to solve inverse problems is, therefore, of major practical and economic importance.

This text is a position paper where we address the relevance of evolutionary computation for iterative approaches to inverse problems. We focus on a set of six real-world problems that we are currently addressing. We assume the premise that the knowledge acquired out of approaching these problems in a coordinated effort will allow us to eventually derive a valuable generic methodology for addressing inverse problems that has evolutionary computation in its core.

After general discussions aimed at providing background material, as well as clarifying our objectives and motivations, we then turn to the inverse problems mentioned above, selected from six areas of science and engineering. The problems are characterised, a description is made of their practical relevance, and a brief explanation is given of the way evolutionary computation appears within each one of them. We will neither discuss any particular problem in depth, nor present any results obtained so far. In fact, our results with these problems are available at varying degrees, since they refer to work in progress. Our emphasis is on the research agenda defined by the problems for the issue of deriving a generic methodology for approaching inverse problems based upon evolutionary computation techniques.

II. Classical Methods

Early inversion methods presented in the literature were empirical or based on highly simplified models, which often failed to capture the essence of the physical problem at issue. Only more recently, the first systematic exploration of the mathematical structure of inverse problems was made (by Backus [3], in the context of Geophysics).

To solve an inverse problem is to infer the values of some of the parameters of a model from a set of measured values of the observable parameters. The main difficulty in tackling inverse problems is due to its intrinsic ill-posed nature, and lies in the fact that the set of measured values often overdetermines some model parameters while leaving others underdetermined.

The classical approach for handling data redundancy is to formulate the inverse problem as an optimisation problem where the objective function to be extremised gives the misfit between the measured values and the simulated results in an Euclidian norm (least-squares method) or in any other appropriate norm (e.g., least absolute value or min-

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imax criterium). Solving the optimisation problem generally involves an iterative search by using a standard minimisation technique such as the conjugate-gradient algorithm or the steepest-descent method. A detailed discussion on the choice of the objective function formulation, based on the statistical description of the measurement errors, can be found in [4]. For a general method for solving multidimensional inverse problems see [11].

Generally, the underdetermination of model parameters are caused by two interconnected reasons: lack of data and experimental uncertainties. It is well known that the presence of noise in the experimental data represents an irrecoverable loss of information that makes a perfect inversion impossible. Therefore, the omission of any prior knowledge about the inverse problem may have serious consequences on its resolution. In other words, observational data is often insufficient to provide a unique and stable solution. The classical approach in this case is to restrict the class of admissible solutions (i.e., the solutions that are consistent with the available data) by using a regularisation term which is added to the objective function by means of Lagrange multiplier. The introduction of a regularisation term into the inversion procedure damps the parameter variability to such a degree that the final solution looks physically acceptable, without (or with a few) artifacts or any other spurious structure. Jaynes [12] proposed the Maximum Entropy (ME) principle as a general inference procedure on the basis of Shannon's axiomatic characterisation of information. Since the end of the sixties, the ME principle has been successfully applied as a regularisation technique to a variety of fields including astronomy, tomography, image restoration or crystallography. Recently, a novel approach for an entropy-based regularisation technique has been proposed by Ramos and Campos-Velho [15].

III. Classical Iterative Methods

Although the classical techniques used today for solving inverse problems are as multifaceted as the problem themselves, it is possible to regard those methods in terms of two classes. As stated by Tarantola [1988], one class "concerns problems where the data and the unknown set can be related by an inversible (generally nonlinear) application", very much "the usual mathematical sense of the word inverse". The members of this class are characterised by this author as exact methods. Considering that in general these methods cannot deal with data uncertainty and data redundancy in a natural manner, they are not relevant for present purposes.

Members of the other class, however, avoid the exact inversion by relying on an optimisation framework to iteratively and locally probe the solution hyperspace by solving a sequence of direct problems until the best (the optimal) alternative is found. Let us refer to the latter as classical iterative (CI) methods. In this class of inversion methods, noise and prior information are easily handled by means of regularization functions or operative constrains. Morever, CI techniques yield the only systematic and sufficiently general methodology for dealing with complex, real-world nonlinear problems in many branches of science and engineering. The major drawback of the CI technique comes from the local nature of the search procedure for the optimal solutions. For large and complex inverse problems the computational effort may become rapidly prohibitive for any practical application, and the risk of the search being trapped in local minima may become unsurmountable, unless a good starting point is available. Clearly, classical methods operate locally, and are not intrinsically parallel.

Under the light of the discussions above, glimpses of a research agenda regarding CI methods can already be perceived.First, one should investigate and improve CI methods, together with new regularisation approaches, for tackling inverse problems. As recalled in [14], a large set of inverse problems in various relevant fields (such as Oceanography) remains unsolved even for classical iterative methods, thus still providing a challenging research agenda. Second, it is worth setting up a large data base of numerical experiments, using CI methods, for validating evolutionary approaches. And third, it is also valuable the provision of a systematic approach for choosing between competing solutions by using entropy-based and other regularisation techniques.

Our point here is, although some of these aspects find their existence within the issue of inverse problems alone, they should not be constrained by that. In fact, the great challenge for present purposes is to generate a new class of hybrid solution schemes integrating evolutionary computation, standard iterative inverse methods, and regularisation techniques.

IV. Evolutionary Algorithms and Iterative Methods

In order to cope with the demands of efficient search within the solution spaces in classical iterative methods, as well as among the solution spaces themselves, a class of search techniques that comes to mind are certainly the evolutionary algorithms (EAs).

Therefore, the role of the EAs are thus on the minimisation of the DISTANCE between a candidate solution of the problem (worked out through the direct model) and the observed value of a variable. For instance, in the example mentioned earlier (where the inverse problem is the determination of the source of an electromagnetic signal on the surface of the earth, by means of its Doppler shift as measured by a satellite in orbit) an evolutionary approach would have the EA minimising the difference between a particular observed Doppler shift and the Doppler shifts that the candidate positions of the source would entail at the satellite, the latter given by the direct model of the situation.

There has been a recent surge of interest in applying evolutionary algorithms to complex combinatorial optimisation problems; see, for instance, [9], [2] and [18]. This is largely due to the robustness afforded by the method, something lacking in traditional operations research techniques. In other words, EAs are able to find good solutions over a wide range of problem instances whereas more traditional techniques must rely on heuristics which are very difficult to make sufficiently broad in scope. EAs are proving themselves to be an important programming methodology for distributed and massively parallel computers, a technology to which they naturally lend themselves.

An additional advantage of this approach is that it has recently been recognised that EAs can be further extended to a class of more ill-posed problems where the number of parameters is not predetermined. In the optimisation of shapes, such as aerofoils, the number of parameters needed to determine any particular shape varies according to how simple or complex it is; similarly for optimising the topology of neural-like networks where the number of nodes is not fixed. Many inverse problems fall into this more difficult category, which we can refer to as inverse design. We have included in our list of selected problems (to be characterised below), one that is certainly of this type (the one about heat-transfer). But it is worth mentioning that the use of variable-length genotypes does not necessarily entail inverse design, as [21] is an example.

This class of open-ended problems poses two major challenges to standard evolutionary methods, and GA in particular. Potential solutions for evaluation are typically encoded on a linear genotype, and the GA uses a population of such genotypes. If the number of parameters in the problem is fixed, then the genotype length will be constant, and the genetic manipulations of the GA are relatively straightforward. However in the case of open-ended problems where the parameter set is variable in number, this requires genotype lengths to also be variable. It turns out that this has significant effects on GA operation, and the necessary modifications to GA practice have been worked out in the SAGA system ([10]). The second challenge arises where there are symmetries in the solution which have to be defined in the genotype by some compact encoding ([5]), and then be decoded back when needed.

A final aspect in regard to evolutionary algorithms that is worth mentioning is the possibility of using hybrid approaches using EAs and standard iterative methods for solving a particular inverse problem. These cases would involve an initial stage based in evolutionary computation, followed by a stage based on traditional methods that would take the outcome of the evolutionary process as a first-guess, from which a standard, specific method would then procceed. The evaluation of this kind of hybrid approach is certainly important, insofar as it can represent an improvement in performance of the search process.

Considering the natural way in which EAs and inverse problems fit together, it is surprising that the explicit connection between them in the literature are relatively rare. And even when it happens, it is usually in very specific attempts, such as in seismology ([19]), acoustics ([7]), and in electromagnetics ([20] and [21]). So far, we have been unable to find a single reference discussing evolutionary algorithms and inverse problems with the breadth of scope we are concerned about herein.

V. A Rich Sample of the Space of Inverse Problems

In order to achieve our objectives we set out to propose solutions to a selected set of real-world inverse problems of various kinds and domains, and compare these results with current approaches whenever applicable. Most of the problems have readily available data.

But let us make two caveats. First, we are not making the point that we will exhaust the knowledge associated with any of the problems below; rather, our intention is to address them and propose new solutions emphasising our chosen approach. Second, although we have already considerably advanced our knowledge about the problems, some details are still missing, with different degrees depending on the problem.

What follows is a list of the problems we have defined, where, for each case we provide the scientific domain in which it appears, a definition of the problem, its relevance, and a brief explanation of the way evolutionary computation can appear in it.

A. *Space Dynamics*

Discovery of the position of drifting data collecting platforms over the Brazilian territory.

Relevance: Brazil's National Institute for Space Research (INPE) has a large array of data collecting platforms over the Brazilian territory and also provide support for private companies to mantain their own platforms. The data collected by the platforms are transmitted to a satellite in orbit which, in turn, relays them back to the ground, where they can be used. These data items are environmental and meteorological data of a local region in the country, thus being important for environmental research, for feeding numerical models in weather forecast, and for various forms of decision making with great economic impact. The problem arises when the platform is mobile, like when it is drifting, say, over the ocean, and therefore, the precise position of the platform is unknown. Attempts to solve this problem at INPE based on standard orbital dynamics models have not yielded a satisfactory result so far.

Direct problem and objective function: The direct method is drawn from [1] and uses the orbital attributes of the satellite, that is, its position in regard to the centre of the Earth, and its speed); the Doppler deviation measured by the satellite; and the expected Doppler deviation that should have been measured by the satellite for the candidate DCP. The model can also account for the existence of ionospheric interference. We have obtained preliminary results on this problem with synthetic data under ideal conditions ([6]), whose evolutionary approach is based on a previous method we developed for another purpose ([8]). The satellites to be considered in this problem are SCD-1, the first Brazilian satellite, and later on, SCD-2, to be launched next year.

To each candidate position it is possible to calculate the expected Doppler shift. The objective function is then defined by the difference between the latter and the actual shift measured at the satellite. In fact, for technical reasons beyond present purposes, we have to include in the objective function the Doppler shift differences of at least two distinct positions of the satellite.

B. Materials Science

Tomographic reconstruction of structural faults in composite samples from scanned surface temperature data.

Relevance: During the past decades, composite materials have found many important applications in various industrials fields (e.g., aerospace, nuclear, micro-electronics). The increasing requirements for assuring the integrity of composite hardware call for appropriate and efficient nondestructive evaluation techniques.

Direct problem and objective function: The associated direct problem involves the determination of the transient temperature response of the composite sample when its internal morphology is known and the initial and boundary conditions are properly specified. It is solved numerically by the finite analytic (FA) method, using an alternating direction implicit scheme ([16]). The basic idea of the FA method is the introduction of local analytic solutions of the governing equation into the numerical solution of the global boundary-value problem.

The objective function gives the misfit in a least-squares sense between simulated and experimental surface temperature data. Due to the presence of noise in the measurements an entropy-based regularisation term is added to the objective function by means of a Lagrange multiplier.

C. Geophysics

Reconstruction of geoelectric conductivity profiles from knowledge of the magnetic field fluctuations at the surface of the earth.

Relevance: This problem, also called magnetotelluric inversion, appears in various areas such as petroleum prospection, mining, and search for underground water. It is of great relevance to the exploration of regions which are difficult to probe with conventional seismic methods.

Direct problem and objective function: The direct model solves the Maxwell's equations with suitable boundary conditions for a given two-dimensional conductivity distribution. The variation with frequency of the electromagnetic fields are computed by finite differences over a nonuniform mesh, according to procedure proposed by Jones [13].

The objective function is defined as the RMS difference between the experimental data and the surface field calculated by the direct model for a given conductivity distriibution. Considering that observational data is insufficient to provide a unique and stable solution, a regularisation term given the entropy measure of the first-differences vector of the problem parameters is added to the objective function ([15]).

D. Heat Transfer

Determination of the optimal geometry and/or internal morphology of two-dimensional arrays of homogeneous media in order to achieve a desired thermal behavior (e.g., a given macroscopic thermal conductivity or a specified heat flux boundary condition).

Relevance: Inverse thermal design problems arise in many areas of engineering and tipically involve an iterative optimisation scheme to achieve the design goal from an initial configuration. Examples include the optimal design of turbine blades, cooling of electronic equipment and management of thermal systems.

Direct problem and objective function: The direct problem gives the transient temperature response of an assembly of two homogeneous media, in perfect thermal contact, with an arbitrary two-dimensional geometry and boundary conditions of the second or third kinds. The diffusion equation is solved by an explicit finite difference numerical scheme over an uniform rectangular mesh. The objective function is chosen according to the design goal to be achieved such as an optimal macroscopic thermal conductivity or a minimal heat flux on the boundaries.

E. Oceanography

Estimation of inherent optical properties (IOPs) distributions in natural waters (e.g., the absorption and the scattering coefficients) from remote sensing data and/or in situ radiometric measurements of underwater light fields.

Relevance: The knowledge of IOPs underwater profiles is of capital importance in the study of biological, chemical and geological components of natural waters and their connection with the physical environment.

Direct problem and objective function: The direct model applies the invariant imbedding method ([14]) to solve the radiative transfer equation for a given set of IOPs and atmospheric conditions. The direct model output includes the complete underwater radiance field and the remote-sensing reflectance. The objective function is computed from the square differences between the direct model output for a candidate solution and the actual remote sensing and/or in situ radiometric measurements.

F. Meteorology

Estimation of temperature and moisture vertical profiles in the earth's atmosphere from microwave and infrared data obtained by the TIROS-N/NOAA satellites.

Relevance: Reconstruction of atmospheric temperature and moisture vertical profiles provides an important input for weather forecast models, mainly in the Southern hemisphere.

Direct problem and objective function: The direct model solves the radiative transfer equation in the atmosphere for known temperature and moisture conditions. The microwave and infrared radiances that reach the satellite sensors are the outputs of the direct model. The objective function is computed from the square differences between the direct model output and the remote sensing data.

Summing up, the problems we have chosen are sufficiently well-defined for being tackled with evolutionary optimisation techniques, and, in some cases, with alternative solutions readily available for performance comparisons. Most important of all, the problems are far from being trivial and their associated direct models yield a wide structural diversity, thus providing a rich sample of the space of inverse problems.

VI. Concluding Remarks

Our approach towards a generic methodology for solving inverse problems relies on iterative methods. The use of evolutionary algorithms, as a viable and general optimisation technique for solving inverse problems seems to be extremely appropriate. Their robustness, ability to perform global search, and potential parallelism, are the major advantages over classical, essentially local methods.

The use of regularisation techniques (mostly entropy-based) as a way to choose between competing solutions of the inverse problem is an important technique for reaching a good solution, regardless of the iterative method being used. In particular, the integration of regularisation methods with evolutionary algorithms is both novel and promising.

Another potentially fruitful proposal we are making is the possibility of generating hybrid solution schemes combining standard, local-based iterative optimisers with the evolutionary approach. The idea is to allow the latter to initially perform a global search in the space of possible solutions (thus reducing it), such that the former would then proceed through a local search over the reduced space obtained out of the initial stage. The additional possibility of incorporating regularisation also in this hybrid scheme might be an extra advantage.

The criteria and procedures to be used for accompanying this research agenda, as well to evalute its success are the following:

1. To achieve a speed-up in the resolution of some inverse problems over existing methods. This criterion applies, for instance, for the geophysics problem, for which we have another resolution method promptly available.
2. To show feasibility of solving problems whose solution is otherwise either not feasible or unpractical at present. The most likely problem in this case is the oceanography problem, whose solutions currently available are still very poor.
3. To generate solutions that lend themselves to parallel implementations, even if their current implementation in serial machine is outperformed by existing methods.

By addressing a rich set of complex, real-world problems we intend to learn about the effectiveness of the techniques we discussed, so as to give a step forward towards a wider-scoped methodology for addressing inverse problems. Such a methodology would certainly be of value in the absence of a more specific approach to a particular inverse problem.

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