Geometric invariants for initial data sets: analysis, exact solutions, computer algebra, numerics

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Abstract. A personal perspective on the interaction of analytical, numerical and computer algebra methods in classical Relativity is given. This discussion is inspired by the problem of the construction of invariants that characterise key solutions to the Einstein field equations. It is claimed that this kind of ideas will be of importance in the analysis of dynamical black hole spacetimes by either analytical or numerical methods.

1. Introduction
Gaining control over the dynamics of black hole spacetimes is one of the great challenges of modern classical General Relativity. This ambitious programme can only be successfully addressed by means of a "multidisciplinary" approach which combines ideas and notions from diverse areas of Relativity and beyond. In particular, very much of what we expect to be able to learn about the behaviour of dynamical black holes will depend on a successful interaction between the two strands of research generically known as numerical and mathematical Relativity. Broadly speaking, numerical Relativity can be understood as the endeavour of solving the Einstein field equations in computers by means of numerical schemes. Similarly, mathematical Relativity can be described as the analysis of solutions of the Einstein field equations by means of analytical methods.

In the last decade mainstream mathematical Relativity has focused on the analysis of the Einstein field equations by means of abstract methods to obtain a wide variety of existence and uniqueness theorems. There is, however, another line of research in mathematical Relativity which is of potential great value for the analysis of dynamical spacetimes: the construction of exact solutions and their characterisation.

The study of exact solutions of the Einstein field equations is a mature subject. The highlights of this programme can mostly be found in the monograph [1]. It is very unlikely that solutions of fundamental physical relevance will be found in the future. Given this state of affairs, it is natural to ask what can one do with this wealth of information that has been extracted from this programme. In this contribution I want to argue that key to exploit these ideas is bringing to the fore a closely related line of research —namely, the analysis of invariant characterisations of spacetimes.
The need for invariant characterisations for solutions to the Einstein field equations stems from the diffeomorphism invariance of the theory. Given two metrics, one can ask whether they are locally isometric—that is, if there is a coordinate that brings one metric to the other. The latter is usually known as the Equivalence Problem, and it was formally solved by Cartan who gave a prescription to answer the question—this prescription involves the computation and comparison of higher order derivatives of the Riemann tensor. Instead of using Cartan’s procedure, one could also address the same problem by means of invariant characterisations—that is coordinate and gauge independent labelling of solutions to the Einstein field equations.

Here I want to argue that methods inspired from the invariant characterisation of spacetimes can prove extremely valuable in the analysis of black hole spacetimes. To see why, I turn my attention to some of the paradigmatic (open) problems in the analysis of black hole spacetimes. For this, let us first recall that the 2-parameter Kerr solution (which includes the Schwarzschild solution as special case) is the prototype of a rotating black hole spacetime in vacuum—its parameters correspond to the mass and angular momentum of the black hole. In this regard, it is strongly conjectured that all stationary vacuum black hole solutions are described by the Kerr family of solutions this problem is called the uniqueness of the Kerr spacetime. In principle, it should be possible to use the Kerr solution to model the exterior of a rotating massive body other than a black hole. This expectation, however, has not been realised and it is now conjectured that there is no perfect fluid configuration whose exterior is described by the Kerr solution—this problem is called the non-existence of an interior for Kerr. The Kerr spacetime is believed to describe, in some sense, the asymptotic state of the evolution of dynamical black hole spacetimes this is sometimes called the consensus view on black holes, and it provides the connection with Cosmic Censorship. Furthermore, black hole solutions which are, in some sense, close to a member of the Kerr family are expected to have the same global and asymptotic structure as Kerr black holes the so-called non-linear stability of the Kerr spacetime.

Although this list does not intend to be extensive, it helps to understand what is, in my opinion, the key problem in the study of dynamic black holes: to understand the role of the Kerr spacetime in the space of solutions to the vacuum Einstein field equations.

2. The Cauchy problem in General Relativity and Computer Algebra

In order to study generic properties of a wide classes of spacetimes, one needs a systematic procedure to construct and parametrise solutions to the Einstein field equations. The Cauchy problem in General Relativity—in which one prescribes some initial data on a some 3-dimensional hypersurface and then purports to reconstruct the spacetime arising from this data—provides a way of doing this. The Cauchy problem (and variations thereof) provide the starting point of not only analytical studies of the Einstein field equations but also of the numerical computation of solutions thereof.

In order to see what it is involved in the Cauchy problem, recall that the Einstein equations are tensorial equations valid in any coordinate system. As such, they cannot directly be identified as belonging to any of the three main families of partial differential equations (hyperbolic, elliptic, parabolic). In order to obtain partial differential equations one has to break the covariance of the equations by picking a direction along which to follow the evolution of the spacetime. Sometimes the peculiarities of the particular problem at hand suggest a natural way of doing this, but very often this choice is essentially arbitrary and only justified by its value in extracting information about the solution in question. The choice of of the direction of time (time vector) needs to be complemented with an election of coordinates. One then speaks of a gauge choice. More generally, and depending on the formulation of the Einstein field equations one is considering, a gauge choice must not be restricted only to a choice of time vector and coordinates, but can
involve further considerations like the choice of a vector frame, a spin dyad or a conformal factor (conformal gauge).

Once the gauge has been fixed, one then proceeds to decompose the Einstein field equations along directions longitudinal and transverse to the time vector to obtain a 3+1 decomposition (or formulation) of the Einstein field equations. Generically, one finds that a certain subset of the resulting equations are intrinsic to the leaves of the foliation implied by the time vector—these are called constraint equations. The other part of the field equations gives describes the evolution of the various field quantities—the so-called evolution or propagation equations. Depending to the type of gauge being used, it may be necessary to supplement the propagation equations with evolution equations for the gauge. The justification behind the approach is as follows:

(i) One first solves the constraint equations on some initial hypersurface.

(ii) On a second step one solves the evolution equations on some neighbourhood of the initial hypersurface.

(iii) Finally, one shows that by virtue of the propagation equations, the constraint equations are satisfied on the same neighbourhood where the propagation equations have a solution.

This last step is usually called the propagation of the constraints.

The algebraic complexity of the Einstein field equations has made the analysis of 3+1 decompositions make the study of 3+1 decompositions of the Einstein field equations a topic where the modern capabilities of Computer Algebra systems have made an impact. One can go a step further: the use of Computer Algebra methods is a key ingredient if one is to fully exploit the potential of the Cauchy problem in General Relativity. The reason behind this assertion lies in the intrinsic nonuniqueness of 3+1 decompositions of the Einstein field equations. As it will be discussed in the sequel, the relevance of Computer Algebra resides not only in the ability to streamline or automatise tedious computations, but in the insight it provides on the structures underlying large and complex systems of equations.

3. Characterising initial data sets

One of the main challenges posed by the Cauchy problem in General Relativity is how to prescribe physically relevant data for the evolution equations. This task is made difficult by the fact that the data has to satisfy the constraint equations. Traditional approaches to the solution of the constraint equations have favoured analytical simplicity over physical considerations—like in the case of conformally flat initial data sets. It is only recently, that more physically realistic initial data sets to describe, say, dynamical black hole spacetimes have been brought to the fore.

As mentioned before, the Schwarzschild and Kerr spacetimes play have a fundamental role among the class of black hole solutions to the Einstein field equations. This point of view is supported on the theoretical side by what Penrose called the establishment’s point of view—see e.g. [2]. From a more applied perspective, this point of view is strongly supported by the numerical simulations of dynamical black hole spacetimes. Hence, it seems of crucial importance to understand what it means that a certain initial data set for the Einstein field equations is data for the Schwarzschild or the Kerr spacetime. Notice that although the Schwarzschild and Kerr solutions have certain symmetries which in a certain sense almost fully characterise them, the existence of these symmetries can be hard to detect on a particular hypersurface of the spacetime.

I formulate the problem of characterising initial data sets for the Schwarzschild or Kerr spacetimes as follows: to provide conditions on an initial data set for the Einstein field equations so that its development is isometric to the Schwarzschild or Kerr spacetimes.
A priori, there seem to be many ways to address this problem. One can think of providing local or global conditions. Furthermore, the conditions can be given in terms of implicit conditions on the data or they can be provided in the form of an algorithm so that they can be explicitly verified. The choice of a particular approach depends very much on the particular applications one has in mind.

Before proceeding to discuss a strategy to attack the problem posed in previous lines, I want to point out that although this programme arose first as an attempt to bridge the gap between analytical and numerical considerations —where a resolution of the problem is of clear interest—it now seems to be also of relevance in providing alternative formulations (and hopefully alternative solutions!) to the paradigmatic problems of the mathematical theory of black holes. A further area of potential analytical and numerical interest is that of the construction of initial data sets for the Schwarzschild and Kerr spacetimes with particular geometric properties. For example, there have been attempts to construct initial data sets for the Kerr spacetime which are conformally flat—it now has been shown that these do not exist [3, 4]. Similarly, it is of interest to see whether it is possible to construct boosted initial data sets for the Schwarzschild spacetime which are maximal.

4. A strategy to characterise initial data sets for the Kerr spacetime

A consequence of the 4-dimensional nature of spacetime is that invariant characterisations of spacetimes are, in general, easier to obtain and formulate than characterisations of arbitrary slices of the spacetime. Accordingly, the approach to obtain a characterisation of data for the Kerr spacetime I want to advocate here is based on the following strategy:

(i) Look for a suitable characterisation of the Kerr spacetime.

(ii) Perform a 3+1 decomposition of the characterisation on an arbitrary slice of the spacetime. Some of the equations thus obtained will be intrinsic, while some others will describe the evolution of the characterisation. From the formed one obtains necessary conditions for an initial data set to be Kerrian.

(iii) Find further assumptions that ensure that the necessary conditions obtained in step (iii) propagate—that is, if they are satisfied on an initial hypersurface, then they are also satisfied at later times so that the spacetime characterisation of the Kerr spacetime is recovered. This step gives sufficient conditions.

Step (ii) in the aforementioned procedure is analogous to the 3+1 splitting of the Einstein field equations into constraints and evolution equations. In a natural way, Computer Algebra methods are of great value here. However, their relevance comes truly to the fore when analysing the interdependences of the various equations arising from the decomposition—ideally, one would like to obtain a minimal set of conditions. Step (iii) is, in turn, analogous to the problem of the propagation of the Einstein constraint equations. This is the most difficult part of the approach. It requires the construction of suitable evolution equations for the necessary conditions obtained in (iii). The use of Computer Algebra is essential in this particular step.

5. Characterising the Kerr spacetime

Several approaches to the problem of characterising the Kerr spacetime have been given in the literature. Each with their own advantages and disadvantages. Here we briefly mention some of these.

a. The Simon and Mars-Simon tensors. A convenient way of studying stationary solutions to the Einstein field equations is through the quotient manifold of the orbits of the stationary Killing vector. The Schwarzschild spacetime is characterised among all stationary solutions by the vanishing of the Cotton tensor of the metric of this quotient manifold—see e.g. [5]. In
a suitable generalisation of the Cotton tensor of the quotient manifold was introduced —the Simon tensor. The vanishing of the Simon tensor together with asymptotic flatness and non-vanishing of the mass characterises the Kerr solution in the class of stationary solutions. In [7, 8] a spacetime version of the Simon tensor was introduced —the so-called Mars-Simon tensor. The construction of this tensor requires the a priori existence of a Killing vector in the spacetime. Accordingly, it is tailored for the problem of the uniqueness of stationary black holes. The vanishing of the Mars-Simon tensor together with some global conditions (asymptotic flatness, non-zero mass, stationarity of the Killing vector) characterises the Kerr spacetime.

b. Characterisations using concomitants of the Weyl tensor. A concomitant of the Weyl tensor is an object constructed from tensorial operations on the Weyl tensor and its covariant derivatives. An invariant characterisation of the Kerr spacetime in terms of concomitants of the Weyl tensor has been obtained in [9]. This result generalises a similar result for the Schwarzschild spacetime given in [10]. These characterisations consist of a set of conditions on concomitants of the Weyl tensor, which if satisfied, characterise locally the Kerr/Schwarzschild spacetime. An interesting feature of the characterisation is that it provides expressions for the stationary and axial Killing vectors of the spacetime in terms of concomitants of the Weyl tensor. Unfortunately, the concomitants used in the characterisation are complicated, and thus, produce very involved expressions when performing a 3+1 split.

c. Characterisations by means of generalised symmetries. Generalised symmetries (sometimes also known as hidden symmetries) are generalisations of the Killing vector equation —like the Killing tensors and conformal Killing-Yano tensors. These tensors arise naturally in the discussion of the so-called Carter constant of motion and in the separability of various types of linear equations on the Kerr spacetime —see e.g. [11, 12, 13]. In particular, the existence of a conformal Killing-Yano tensor is equivalent to the existence of a valence-2 symmetric spinor satisfying the Killing spinor equation. An important property of the Schwarzschild and Kerr spacetimes is that they admit a Killing spinor. This Killing spinor generates, in a certain sense, the Killing vectors and Killing-Yano tensors of the exact solutions in question [14]. In [15, 16] it has been shown that for a spacetime which is neither conformally flat nor of Petrov type N, the existence of a Killing spinor associated to a Killing-Yano tensor together with the requirement of asymptotic flatness renders a characterisation of the Kerr spacetime. In a further analysis, it has been possible to remove the a priori assumptions on the Petrov type —see [17].

Although at first sight independent, the characterisations of the Schwarzschild and Kerr spacetimes described in the previous paragraphs are interconnected —sometimes in very subtle manners. This is not too surprising as all these characterisations make use in a direct or indirect manner of the fact that the Kerr spacetime is a vacuum spacetime of Petrov type D —see e.g. [1] for a discussion of the Petrov classification. The art in producing a useful characterisation of the Kerr spacetime lies in finding further conditions on type D spacetimes which are natural and simple to use.

6. Using Killing spinors to obtain a characterisation of Kerr initial data

In this section I want to briefly describe the key ideas behind a characterisation of Kerr data based on the notion of Killing spinors. This is a non-technical summary of the ideas exposed in [15, 16, 17, 18]. The reader is referred to these references for a detailed exposition of the topic.

The starting point of the construction is the observation that the existence of a Killing spinor in the Kerr spacetime allows to relate the Killing vectors of the spacetime with its curvature in a neat way. The reason for its importance can be explained in the following way: from a specific Killing spinor it is possible to obtain a Killing vector which in general will be complex. It turns out that for the Kerr spacetime this Killing vector is in fact real and coincides with the
stationary Killing vector. It can be shown that the Kerr solution is the only asymptotically flat
vacuum spacetime with these properties.

Given the aforementioned spacetime characterisation of the Kerr solution, the question now
is how to make use of it to produce a characterisation in terms of initial data sets. For this, one
has to encode the existence of a Killing spinor at the level of the data. The way of doing this was
first discussed in [19] and follows the spirit of the well-known discussion of how to encode Killing
vectors on initial data —see e.g. [20]. The use of Computer Algebra methods is instrumental to
implement these ideas in an effective manner.

The conditions on the initial data that ensure the existence of a Killing spinor in its
development are called the Killing spinor initial data equations and are, like the Killing initial
data equations (KID equations), overdetermined. In [21], a procedure was given on how
to construct equations which generalise the KID equations for time symmetric data. These
generalised equations have the property that for a particular behaviour at infinity they always
admit a solution. If the spacetime admits Killing vectors, then the solutions to the generalised
KID equations with the same asymptotic behaviour as the Killing vectors are, in fact, Killing
vectors. Therefore, one calls the solutions to the generalised KID equations approximate symmetries. The total number of approximate symmetries is equal to the maximal number
of possible Killing vectors on the spacetime. A peculiarity of this procedure is that if the
spacetime is not stationary, the approximate Killing vector associated to a time translation does
not have the same asymptotic behaviour as a time translation.

The Killing spinor initial data equations consist of three conditions: one of them differential
(the spatial Killing spinor equation) and two algebraic conditions. Following the spirit of [21]
we construct a generalisation of the spatial Killing spinor equation —the approximate Killing spinor equation. This equation is elliptic and of second order. This equation is the Euler-
Lagrange equation of an integral functional —the $L^2$-norm of the exact spatial Killing spinor
equation. For this equation it is possible to prove the following theorem:

**Theorem 1.** For initial data sets to the Einstein field equations with suitable asymptotic
behaviour, there exists a solution to the approximate Killing spinor equation with the same
asymptotic behaviour as the Killing spinor of the Kerr spacetime.

The proof of this theorem is based on an adaptation of standard arguments of the theory of
systems of elliptic partial differential equations on non-compact manifolds. In particular it is
necessary to make use of so-called weighted Sobolev spaces. Remarkably, some of the technical
points of the proof require intensive Computer Algebra computations. Again, this type of
methods show their effectiveness as a tool to investigate the properties of large systems tensorial
and spinorial equations.

It should be pointed out that the conditions on the asymptotic behaviour of the initial data
are rather mild and amount to requiring the data to be, in a sense, asymptotically Kerr data.
The precise version of this theorem generalises the one discussed in [15] in that it allows for
boosted data. This generalisation is only possible after a detailed analysis of the asymptotic
solutions of the exact Killing spinor equation.

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1 The computations described in this contribution have been carried out in the suite xAct for Mathematica:
www.xact.es.

2 For a time translation it is understood a Killing vector which in some asymptotically Cartesian coordinate
system has a leading term of the form $\partial_t$.

3 The idea of using the spatial part of spinorial equations to characterise slices of particular spacetimes is not
new. In [22] the spatial twistor equation has been used to characterise slices of conformally flat spacetimes. See
also [23].
The approximate Killing spinor discussed in the previous paragraphs can be used to construct a geometric invariant for the initial data set. This invariant is global and involves the $L^2$ norms of the Killing spinor initial data equations evaluated at the approximate Killing vector. It should be observed that part of the invariant satisfies a variational principle —this is a further difference with respect to the construction of [21]. As the initial data set is assumed to be asymptotically Euclidean, one expects its development to be asymptotically flat. This renders the desired characterisation of Kerr data and the following result.

**Theorem 2.** Consider an initial data set for the vacuum Einstein field equations such that the $L^2$ norm of the Killing spinor initial data equations evaluated at the solution (with the same asymptotic behaviour as the Killing spinor of the Kerr spacetime) to the approximate Killing spinor equation vanishes. Then the initial data set is locally data for the Kerr spacetime. Furthermore, if the 3-manifold has the same topology as that of hypersurfaces of the Kerr spacetime, then the initial data set is data for the Kerr spacetime.

The invariant described in this theorem is a non-negative number having the property that it vanishes if and only if the initial data set corresponds to data for the Kerr spacetime. Thus, the invariant measures the *non-Kerrness* of the initial data and condenses it in a single number. The question whether this invariant constitutes a good distance in the space of initial data sets is currently being investigated.

Keeping in mind possible applications to the numerical simulation of black hole spacetimes, it is worth pointing out that the construction of the invariant is fully amenable to a numerical implementation —the elliptic solvers that one would need to compute the solution to the approximate Killing spinor equation are, nowadays, standard technology.

In view of possible applications of the non-Kerrness to the problem of the uniqueness of stationary black holes and the non-linear stability of the Kerr spacetimes, it is important not only to consider hypersurfaces with two asymptotic ends, but also ones with an inner boundary having the topology of a 2-sphere. This boundary can represent the horizon of a black hole or the surface of a star. Generalisations of Theorems 1 and 2 for 3-dimensional hypersurfaces with the topology of the complement of an open ball in $\mathbb{R}^3$ have been given in [17]. The analysing leading to these generalisations is more technically involved than that of [15, 16] as it requires the verification of certain compatibility conditions on the boundary and the specification of the right boundary value for the elliptic problem. Remarkably, the theory of Killing spinors readily provides a formula for a Killing spinor candidate in terms of concomitants of the restriction of the Weyl tensor of the spacetime to the boundary of the hypersurface —a further connection with the theory of exact solutions to the Einstein field equations.

Further extensions (not yet fully analysed) of the ideas discussed in this section include 3-manifolds with a a cylindrical end (trumpet data) and hyperboloidal manifolds. There are reasons to suggest that the latter can be of particular importance in the analysis of evolution issues.

**7. Concluding remarks**

The purpose of the present contribution has been to highlight the potential that exist in carrying out research following an inclusive point of view that encompasses ideas from exact solutions, analytic methods, computer algebra techniques and numerical simulations.

A natural question concerning the invariants here discussed is that of their behaviour under time evolution. An input from numerical investigations can be of great utility to address this question. Conversely, it is conceivable that the feedback provided by this type of theoretical considerations can have a useful impact in numerical investigations of solutions to the Einstein field equations. If some type of constancy or monotonicity property could be established for the
geometric invariant by either analytical or numerical methods, this would be a useful tool for studying non-linear stability of the Kerr spacetime and also in the numerical evolutions of black hole spacetimes.

Finally, it is worth pointing a further, rather intriguing connection of the geometric invariants I have been describing. Namely, in [18] it has been shown that the construction of [15, 16, 17] mimics several aspects of Witten’s proof of of the Mass Positivity Theorem by spinorial methods —see [24]. The full implications of this connection still awaits a detailed consideration. As in previous analysis, it is very likely that a combination of various techniques coming from traditionally different areas of research in General Relativity will be instrumental to obtain key insights.

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