On ab initio closed-form expressions for gravitational waves

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We introduce an approach for finding ab initio, high accuracy, closed-form expressions for the gravitational waves emitted by binary systems. Our expressions are built from numerical surrogate models based on numerical relativity simulations, which have been shown to be essentially indistinguishable from each other, with the advantage that our expressions can be written explicitly in a few lines. The key new ingredient in this approach is symbolic regression through genetic programming. The minimum overlap obtained in the proof of concept here presented, compared to ground truth solutions, is 90%.

Motivation and Introduction.– The surge of direct detections of the gravitational waves (GWs) emitted by the collision of two black holes and neutron stars through laser interferometer laboratories [1] puts even more demand on the need for fast evaluation of GWs emitted by these processes as well as the collision of neutron stars or mixed pairs, as predicted by Einstein’s theory of gravity or alternative ones [2].

High accuracy numerical simulations of the Einstein equations (EE) are the gold standard for these predictions. The problem is that they are computationally very expensive. As an example, if one considers the case of two black holes, initially far away and in quasi-circular orbit, the usual rationale is that due to the no-hair theorem each hole can be uniquely described by its mass and spin. That is 8 degrees of freedom. The total time of computation (wall time) elapsed for each of these simulations depends on the initial separation of the two black holes. For the sake of definiteness, let’s say that each simulation takes 10,000 hours of wall time, which is a lower bound for cases of interest. Assuming that one samples each parameter dimension with, say, 100 points, either equally or randomly spaced, this gives \(10^{16}\) years of computing time, which is orders of magnitude larger than the age of the universe. Even using the top 10 supercomputers [3] one would reduce this time to \(\sim 10^8\) years. Even worse, for Bayesian parameter estimation, a catalog/bank of templates cannot be constructed a priori since each new waveform needs to be computed on demand without a priori knowledge of which ones those will be [4].

This is a problem that cannot be solved through software optimization or specialized hardware (such as GPUs). This gave rise to the introduction of Phenomenological [5] and Effective One Body (EOB) [6] models. These are not solutions of the Einstein equations but, instead, physically inspired fits or approximate modeling of the EE for binary systems. We will not review these approaches here since our take is to represent the emitted GWs using the full EE, through an ab initio approach. This effort over the last decade motivated the introduction and development of surrogate models which are essentially indistinguishable from numerical relativity (NR) simulations, but with a speedup of evaluation of around eight orders of magnitude [7], with each mode being evaluated in the order of milliseconds on a standard laptop instead of using supercomputers. A relatively small number of NR simulations are still needed in the offline (training) stage, though, but with a fast, highly accurate, surrogate, predictive model to evaluate for any parameter and time in the intervals considered in the online stage.

In this Letter we build upon these efforts for what we consider the next step: a methodology for finding high accuracy symbolic (closed-form) expressions, as opposed to numerical surrogates. As a proof of concept we present results for the system considered in [7].

Surrogate Models.– Surrogate models in general follow different approaches for regression [8] and/or reduced order modeling (ROM) for parameterized systems. Here we focus on the latter, we will not delve into reviewing them but instead refer to [9]. In this work we focus on Reduced Basis (RB) [10–11], the Empirical Interpolation Method (EIM) [12–14], and Symbolic Regression (SR). Briefly, RB collocates parameter points in a nearly optimal way according to their relevance, which are used to build a hierarchical, nearly optimal basis in a rigorous mathematical sense with respect to the Kolmogorov n-width [15–16]. The framework of RB takes advantage of any regularity with respect to parameter variation to achieve fast convergence in the accuracy of the representation with the number of basis elements; it is usually referred to as an application-based spectral expansion. In fact, in the case of gravitational waves it can be easily argued that the parameter dependence is smooth \((C^\infty)\) and RB has been shown to achieve asymptotic exponential convergence [17–23], as expected with any spectral-type method.

On top of that, high accuracy predictive models (pre-
prediction as opposed to projection) can be built once one has a reduced basis and an empirical interpolant [20]. Furthermore, one can achieve a subsampling in the space dual to that of one of parameters (time in the case here considered) which is also nearly optimal, using the EIM in the sense of step by step attempting to minimize the Lebesgue constant. Roughly speaking, this means minimizing the error in the interpolant compared to that one of projection onto the corresponding reduced basis. The availability of high accuracy, fast to evaluate, predictive models and a sparse subsampling in time are key components upon we build on in the approach presented in this Letter for finding ab initio symbolic (closed-form) expressions for GWs.

Symbolic regression using genetic algorithms.— Genetic programming (GP) is, in brief, an area of Artificial Intelligence whose goal is the evolution of programs or tasks through computer means. The techniques of GP emulate those of Nature; that is, algorithms are modeled following the process of natural evolution. A thorough book on GP is [24], and a shorter field guide [25].

Symbolic regression (SR) uses genetic algorithms to find closed-form expressions in an agnostic (data-driven) and unsupervised way, either looking for expressions representing data or differential equations describing them, with the possibility of constraints, either algebraic or differential [26]. SR can be described through the following general tree-structured algorithm tracing genetic programming principles:

1. Create stochastically an initial population of programs (e.g., mathematical expressions and operations);
2. Repeat
3. Execute each program and compute their quality or fitness;
4. Select one or two programs from the population with a probability based on their fitness to participate in genetic operations;
5. Create new programs through the application of genetic operations (e.g., mutation or crossover);
6. Until an acceptable solution is found or some other stopping condition is met;
7. Return the best-so-far individual/s.

In this work we used Eureqa [27] for SR, although there are less developed open source alternatives such as gplearn [28], with the possibility of extensions and improvements. Having said that, there are open source efforts to recreate Eureqa.

It is worth pointing out that SR algorithms do not find a unique representation but a number of them, with different levels of computational complexity (cost of evaluation, for simplicity) and accuracy with respect to training and validation sets. So, depending on the criteria used for finding expressions via SR, the final symbolic forms can be shorter or larger with variable accuracy. In this work we prioritize accuracy.

An example: a robot discovering Newton’s second law.— As an example of the power of SR using GP we present results for the following system: the simple pendulum. In polar coordinates, Newton’s second law is

$$\ddot{\theta} = -g/l\sin(\theta),$$  

(1)

where $g$ is the gravitational acceleration, $l$ the longitude of the pendulum and $\theta$ the angle with respect to the point of stable equilibrium (the pendulum at rest). For given initial conditions, we solved the above ordinary differential equation (ODE) for a number of initial conditions, utilizing standard numerical integrators, and used the resulting data (with intrinsic noise, due to the numerical errors of the ODE solver) to find symbolic expressions for the underlying differential equation, searching for expressions of the form $\ddot{\theta} = f(\dot{\theta}, \theta, t)$ . The representation found with the highest accuracy is exactly, not a numerical approximation of, Newton’s second law for this system, Eq. (1). Furthermore, for initial conditions close to the stable equilibrium state, one of the symbolic expressions found was exactly the harmonic oscillator equation.

Although the following conclusion could be somewhat debatable, the point is that a robot could find Newton’s fundamental second law in seconds. One could argue that it is for a particular system but, though not presented in these terms, this is the process of scientific induction. In data science (DS), machine learning (ML) or artificial intelligence (AI), this process is called validation, whereas in physics it is called verification (as in verifying Newton’s or Einstein’s theory of gravity). In fact, with more computational power, the authors of Eureqa remarkably “discovered” Newton’s second law for the double pendulum, which is known in physics as a classical example of a chaotic system [29].

Method outline.— As a proof of concept here we used the surrogate model of [29], which is part of the publicly available GWSurrogate package [31], to build a set of waveforms to train SR and find symbolic expressions for the whole space considered. That is, those not included in the training set. The model corresponds to the collision of two black holes initially in quasi-circular orbit and without spin, for about $25 - 31$ GW cycles before merger. More precisely, for the time interval $t \in [-2, 750 : 100] M$, where $M$ is the total mass of the system and the waveforms have been aligned so that $t = 0$ corresponds to the peak of their amplitudes. The only free parameter then is the mass ratio $q := m_1/m_2$, in the range $q \in [1, 10]$, with $m_i$ the mass of each black hole. Furthermore, for definiteness we restrict our discussion to the dominant mode, the $\ell = m = 2$ one.

This surrogate model consists of only 22 basis elements and, by construction, only 22 time EIM nodes. These are the only pieces of information needed to predict with high accuracy any waveform in the space considered.

The surrogate model can be considered (and we do) as ground truth solutions of the EE, since it was shown...
in [30] that it is essentially indistinguishable from NR simulations up to the numerical errors of the latter, performed by SpEC [32], the most accurate code in the NR community to date for modeling GWs sources without shocks (such as binary black holes).

The two polarizations of GWs can be encoded in a single complex parameterized function,

\[ h(t, \lambda) := h_+(t, \lambda) + i h_\times(t, \lambda), \]

where \( \lambda \) represents a tuple in parameter dimension; here, it corresponds to the mass ratio \( q \). The waveforms for the collision of two black holes in initial quasi-circular orbit have an apparent complexity, but they are simply oscillatory functions with an increasing amplitude until the time of coalescence, followed by a damped exponentially decaying profile, the quasinormal modes of the final black hole. It is therefore convenient to consider the amplitude \( A(t, \lambda) \) and phase \( \phi(t, \lambda) \) separately,

\[ h(t, \lambda) := A(t, \lambda) \times e^{i \phi(t, \lambda)}, \quad (2) \]

find closed-form expressions for them, later reconstruct the symbolic waves and compare them with their ground truth counterparts for a large number of validation cases.

Results for binary black hole inspirals.– For both amplitude and phase our symbolic expressions have an R squared goodness of fit of at least \( R^2 \approx 0.999 \) with respect to the validation members of the catalog used in the symbolic regression searches. We discuss more thorough and large-scale validation results below.

Amplitude.–

In our experience, naively sampling both in parameter (mass ratio \( q \)) and physical dimension (time) resulted in days or weeks of no convergence while searching for symbolic expressions for the amplitude of the GWs. The reason for this is the need to resolve with high accuracy the region around the peak of the amplitude, for which we tried using a dense sampling in time —up to \( \sim 10^3 \) equally spaced time points—, leading to high computational times for unsuccessful results.

One could attempt to manually collocate time nodes where needed. This approach is not only tedious but not guaranteed to work. Instead, here we resorted to subsampling in time using only the 22 EIM nodes, shown in Fig.1, and 90 equally spaced values in the mass ratio. The rationale for this approach is that the EIM time nodes are the only relevant ones for recovering the whole time series and thus the only representative ones; this intuition proved to be correct, as we discuss below. Using only the EIM nodes in a few minutes we were able to find the following closed-form expression for all \( q \in [1, 10] \) (we discuss validation using a dense set of time nodes below):

\[
A(t, q) = \frac{\{a_1 e^{\text{atan2}(t, a_2-t)}/(a_3 + q - t - a_4 \text{gauss(atan2}(a_5, q) - a_6 t)}\)\} - a_9, \]

where \(\text{gauss}(x) := e^{-x^2} \), \(\text{atan2}(x, y)\) is the arctangent of two parameters and

\[
a_1 = 1.37502533181183, \quad a_2 = 0.0409895367586908, \quad a_3 = 3.40043449934568, \quad a_4 = 1.86434379599601, \quad a_5 = 1.1446516014466, \quad a_6 = 1.49686180948812, \quad a_7 = 0.0250835926883564, \quad a_8 = 0.108134472792241, \quad a_9 = 0.00178301085458751. \]

Phase.– Although we were able to find high accuracy symbolic expressions for the phase in the considered interval of \( q \in [1, 10] \), they resulted in large propagation errors in the reconstruction of the waveforms. The reason is different from phase accumulation errors in numerical relativity, since here we are dealing with global (in time) optimization errors and is simply the following: a change in phase \( \phi \to \phi + \delta \phi \) in (2) leads to an error in the waveforms of the form

\[ h \to \hat{h} := A \times e^{i(\phi + \delta \phi)} \approx h (1 + i \delta \phi), \]

so \( |\delta h|/A = \delta \phi \). In order to get a relative error of 1% at least, we must have an order of 0.01 in the phase error \( \delta \phi \). For the whole \( q \in [1, 10] \) phase symbolic model, in the results here obtained \( \delta \phi \) is of order 1 (with a relative error less than \( 10^{-2} \)), leading to large errors when reconstructing the waveforms.

A simple domain decomposition to solve this issue worked out for us: we subdivided the domain \( q \in [1, 10] \) into 9 equally spaced subdomains of the form

\[ q \in [1, 2], [2, 3], \ldots, [8, 9], [9, 10]. \]

Domain decompositions are standard when solving partial differential equations (PDEs). In fact, it is possible that in more complex scenarios an hp-greedy domain decomposition [33,35] (where the hp term is actually borrowed from domain decomposition and refinement in finite elements when solving PDEs) might be necessary.

For finding symbolic expressions for the phase we used 20 values in mass ratio and 285 time nodes for each domain. The results are publicly available from [37].
Validation and accuracy of symbolic waveforms.— The steps of validation for building surrogate models based on RB and the EIM are described in [17, 18, 20, 30]. So here we focus on the ones related to SR. In this processes we used a fraction of our catalog for training and another one for validation so as to avoid overfitting; typically we used 50% for each (training and validation).

Afterwards we reconstructed, from the symbolic amplitude and phases, the time series for the two polarizations of the GWs and compared them with the ground truth solutions using $10^5$ GWs per each subdomain $[q_i, q_{i+1}]$, $i = 1, \ldots, 9$, and the whole 28,501 time samples provided by GW surrogate, leading to $\sim 10^6$ validation waveforms. This validation instance was achieved by computing the overlap integral $S[h_{\text{sur}}, h_{\text{sym}}](q)$ between surrogate $h_{\text{sur}}^\tau(t, q)$ and symbolic $h_{\text{sym}}(t, q)$ complex normalized waveforms in the time domain, defined as

$$S(h^1, h^2) := \text{Re}(h^1|h^2) = 1 - \frac{1}{2} ||h^1 - h^2||^2,$$

where

$$\langle h^1|h^2 \rangle := \int_{t_{\text{min}}}^{t_{\text{max}}} dt \ h^1(t) \ h^2(t),$$

and $||h||^2 := \langle h|h \rangle$. The overlap $S$ gives a measure of the match between two waveforms and is commonly used in GW science.

The result is that the overlap $S = S(q)$ in our approach gives values above 99% for all cases. The main reason that we could do this a posteriori dense validation is due to the fact that ground truth solutions using surrogate models can be evaluated very quickly, typically in less than a second on a standard laptop. The results are shown in Fig. 2. One should not reach any conclusion from the dependence of the overlap $S$ as a function of the mass ratio $q$, since these are representations, much as in domain decomposition approaches in NR (tough usually in physical space, not in parameters). For example, we could have chosen to show results for symbolic expressions with a more uniform error distribution, though it is worth emphasizing that the differences in the figure are in the order of 0.1%.

As an example, in Fig. 3 we show the ground truth solution on top of its symbolic expression for $h_+$, corresponding to the worst match in the validation space for the whole interval $q \in [1, 10]$. Results for $h_\times$ are similar since both modes are related simply by a $\pi/2$ phase difference.

FIG. 2. Overlap $S(q)$ for the symbolic waveforms vs the mass ratio $q$, when compared to ground truth solutions, using $q \sim 10^6$ values. The minimum and maximum overlaps are $S = 0.9905$ and $S = 0.9986$, respectively. The dotted lines delimit each subdomain $[q_i, q_{i+1}]$ for $i = 1 \ldots 9$.

Outlook.— In perspective, having high accuracy, closed-form (symbolic) expressions for the emitted gravitational waves as predicted by a theory as complex as Einstein’s one of gravity, for a process as complex as the collision of two black holes, without any simplification in the theory (thus the ab initio emphasis), in a completely unsupervised way, cannot be over-emphasized. Our approach is one of the many trends in the gravitational wave science community to incorporate tools from DS, ML and AI, but to our knowledge it is the first of its kind. Because of this, it is difficult to anticipate the impact and ramifications of our approach.

In this sense, our approach might be useful, for example, for other ones combining ROM with Deep Learning for GW inference [38], which produces, and starts with (at least in its current version), closed-form expressions.

We presented a proof of concept for a novel approach. A next natural step might be to apply it to the other multipole modes of [7], and more complex systems such as the case of spinning, precessing black holes using, for
example, the surrogate models of [39–41]. It is possible that for these cases, and higher dimensionality ones in parameter space in general, training symbolic regression using not only the EIM time nodes but also the greedy parameter values to increase sparseness and avoid the curse of dimensionality of SR searches as in this Letter, would be beneficial.

Even though here we have focused on symbolic expressions based on surrogates built from high accuracy numerical relativity simulations, our approach can be applied to other surrogates based on RB and the EIM, for example those based on EOB ones [20, 42].

The sparse yet near-optimal subsampling in time using the EIM is a key ingredient in our approach, so it is not clear that other surrogate models based, for example, on Gaussian regression (see, e.g. [43]) can take advantage of this key ingredient, but it might be somewhat possible.

There might be potential in enriching the dictionary here used for SR (composed of elementary functions and basic arithmetic operations) using phenomenological or other physically based symbolic models. In this sense, using SR should outperform any other kind of physics-based fits by design, with the advantage of being completely unsupervised and counting with fast to evaluate, high accuracy surrogate models for fast and large-scale validations.

In general terms, the approach here presented should be applicable to other disciplines beyond gravitational wave science since computational complexity is a common problem in genetic programming.

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