Determining remnant parameters from black-hole binary systems
Interim Report 1 - LIGO Document T1700339

Nicholas Meyer[1] and Mark Scheel[1]

[1] *Theoretical Astrophysics 350-17, California Institute of Technology, Pasadena, CA 91125, USA*

(Dated: July 12, 2017)

MOTIVATION FOR PHENOMENOLOGICAL FITS AND METHODS OF FOCUS

The detection of gravitational waves by the advanced LIGO interferometers [1] represents a confirmation of a substantial prediction of Einstein's theory of general relativity. This discovery has additionally established gravitational waves as a new source of data from which information about the observable universe may be obtained.

Of particular relevance is the use of gravitational-wave data to estimate the parameters (masses and spins) of mergers of black-hole binary systems. For this purpose, it is often beneficial to predict the post-merger mass, spin, and recoil velocity as a function of the initial mass ratio and spins of the binary. For example, the SEOBNRv3 waveform model [2] used for LIGO data analysis uses such a prediction of the post-merger mass and spin to compute the ringdown portion of the waveform. Predicting the parameters of the remnant black hole requires numerical relativity simulations, and exhausting the input parameter space through direct simulation is not tractable. Formulas for these final parameters which approximate the values given by numerical relativity are useful because they provide a procedure for obtaining final parameter values at a continuum of initial parameter inputs at a lower computational cost.

To address this need, phenomenological fits of final parameters as functions of initial parameters have been developed by several efforts for the case of aligned spins [3, 4] and some cases of generic and precessing spins [5, 6]. Our goal is to expand upon this work using a new set of over 1000 simulations of binary mergers from the SXS public and incoming catalogs [7], improving upon the formulas particularly in the case of generic spins and exploring the use of general machine learning methods to obtain fits.

We hope to see improvement from two angles: first, from fitting to a newer and larger set of black-hole binary simulations. And second, from new approaches to fitting the results of the simulations. In particular, we evaluate the suitability of neural nets and gaussian process regression for remnant parameter fits.

It will be important to compare the error of new fits obtained for these runs with those of previous studies. A relative advantage of newly obtained fits with respect to error will serve as a measure of success of the project.

An objective is to release public code with subroutines to compute the fits obtained in the analysis. This will be key to allowing these results to be easily replicated and used in further work.

EVALUATION OF MACHINE LEARNING APPROACHES

In order to assess the feasibility of fitting the SXS data with neural net and gaussian process regression, we first perform fits to a known analytic function. This allows us to determine how many sample points are needed to fit this function to a given level of accuracy. For our analytic function, we chose the formula in Ref. [8] for the remnant mass of the black hole as a function of the masses and spins of the two binary components. The inputs for this function include only spin directions aligned with the orbital angular momentum. Because the form of the fits for generic spin should reduce to this case for aligned spins, this exercise serves as a proxy for how well the methods should be able to fit data from actual numerical relativity simulations (the number of input features for the general fits from the SXS catalog is greater than that of this exercise, meaning the fitting error from this exercise is likely a lower bound on the fitting method error). In particular, the formula in Ref. [8] is inexpensive to compute, and so an arbitrary number of points can be generated to examine how errors converge with available data.

Fits were performed in python, using modules from the scikit-learn (`sklearn`) package. When fitting all models, data is partitioned into a subset for fitting or training, and another subset for validation of the results using the function `sklearn.model_selection.train_test_split`. Examination of the fit residuals on the validation set, which is not used in fitting the model, provides a good estimate of the error that should be expected when evaluating the trained model on new data.

Neural Nets

The class used for neural net regression was `sklearn.neural_net.MLPRegressor`.

Sets of 10^3, 10^4, and 10^5 input parameters (spin1, spin2, mass1, mass2) were randomly generated and partitioned into training and validation sets, and the remnant mass of each point was computed according to the formula in Healy and Lousto [8]. A neural net regressor was constructed with various hidden layer sizes and fit to the training set. The relative errors for 10^3 points was around 3% for training and 4% for validation. For 10^4 points, the error was around 2% for both training and validation, and for 10^5 points the error for training and validation were within around 0.8%.

The errors for the remnant mass and spin for the analytic formula used to generate the output values were of the order $\sim 0.2\%$ [8], which is an order of magnitude lower than the error obtained with 1000 points (similar to what is available in the SXS simulation catalogs). From this, neural net regression did not appear promising enough to use in actual fits.

Gaussian Processes

The class used for gaussian process regression was `GaussianProcessRegressor` from the `sklearn.gaussian_process` module.

In contrast to neural net regression, a gaussian process regressor constructed with default parameters recovered the remnant mass formula in Ref. [8] to within 0.05% error using 1000 points for training and validation.

This error is substantially lower than the desired 0.2% threshold for this exercise, and so gaussian process regression appears to be adequately suited to learning on 10^3 data points.

REGRESSION ON NUMERICAL RELATIVITY SIMULATIONS

Our ultimate goal is to fit the remnant mass, spin, and recoil as a function of all seven input parameters in the case of generic spins. As a first step, we fit the remnant mass for the case where the initial black holes have zero spin. For this first exercise, the gaussian process regression class provided by `sklearn` is used to perform the fit. Next, we will treat the case where the black holes have spins aligned or anti-aligned with the orbital angular momentum and compare this with [8]. After this, we will address the general seven dimensional problem.

Upon promising results from the above proof of concept, gaussian process regression was used to fit the final remnant mass in the case of spinless initial black holes. The resulting fit and residuals are summarized in FIG. 1 and FIG. 2. From the residuals it can be seen that the error in the fit is within 0.1% for all simulations. From the plot of the final mass against the relaxed mass ratio of the initial black holes, it can be seen that the best value fit appears smooth and should interpolate well for input mass ratios between 1 and 10.

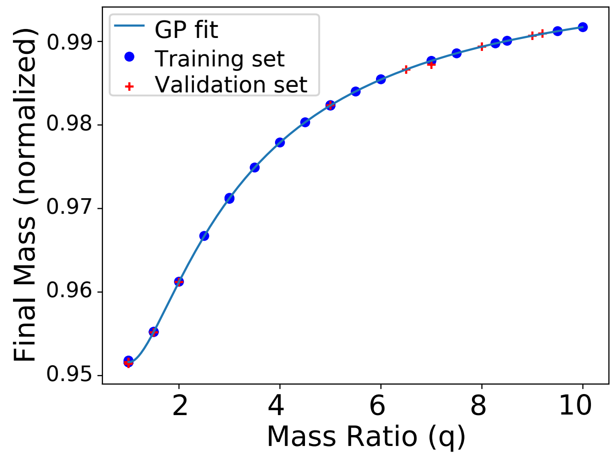

FIG. 1. Plot of predicted remnant mass (solid curve) from gaussian process regression fit, with training data set (solid dots) and validation set (plus signs) overlayed. The training set was used to fit the gaussian process model, while the validation set was used only in assessing residuals. Fitting was performed on the relaxed masses of each input black hole (two input features). The 49 data points (randomly partitioned into 37 training, 12 validation) were selected from the public and incoming SXS catalogs by selecting all simulations for which the square of the initial dimensionless spin magnitude was less than 10^{-10} for both black holes. Note that the mass ratio can be similar between different simulations, and so some points at certain mass ratios represent more than one training or validation simulation.

CHALLENGES

Implementation of Previous Fits

It was necessary to manually implement the fits in Ref [8] in python. Using the `astropy.table.Table` class, it was possible to import formula parameters from the tables in the latex source of the paper.

In order to ensure that the work done in this project can be quickly replicated, python code for computing fits and generating plots will be released to the public along with the final report.

Package Management

Package management of python modules on the `wheeler` machine used by SXS has presented some challenges. The class `sklearn.gaussian_process.GaussianProcessRegressor`, which is necessary for the gaussian process regression code, is present only in `sklearn` version `0.18.1` and above; `wheeler` has version `0.17.1` installed system-wide using the default python environment.

To obtain an updated version of `sklearn`, a custom

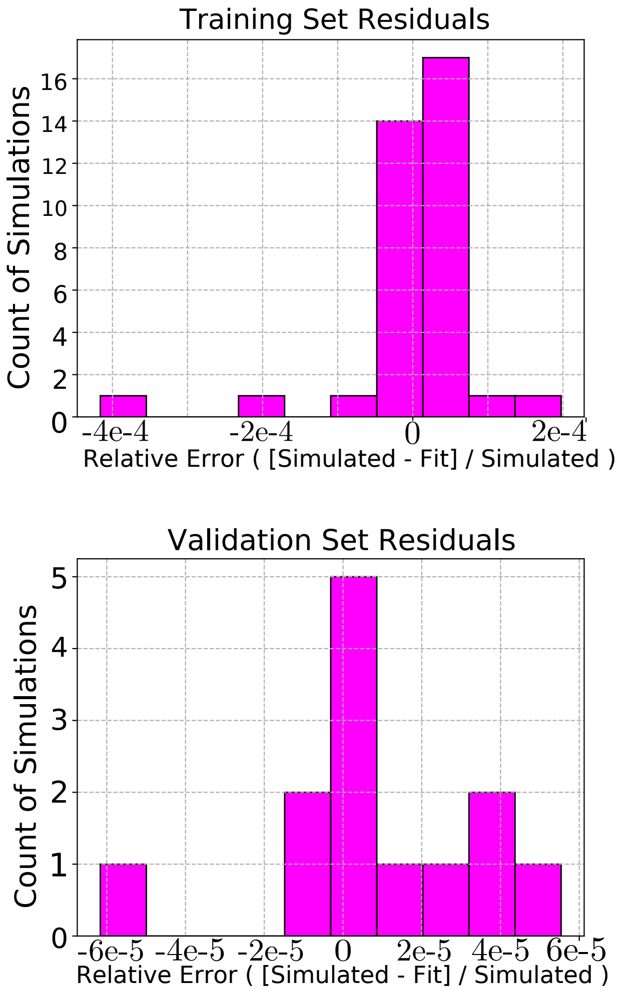

FIG. 2. Training set residuals (top) and validation set residuals (bottom) for a gaussian process fit of the spinless data. Here 36 randomly selected training points were used for the fit out of the 49 spinless simulations, and the remaining 13 formed the validation set. The histogram bins are divided into ranges of relative errors, and the height of each bar corresponds to the number of simulations for which the error lies within the bin boundaries.

local root was created using the conda package manager using the following commands:

```
conda create -n name_of_local_root \
--clone=/anaconda/install/directory
source activate name_of_local_root
conda remove conda-env
conda update anaconda
```

GOALS

A goal of the first portion of the project time was to evaluate the viability of fitting methods and proceed with those which showed promise. Based on initial exercises, gaussian process regression shows much promise for fitting the generic spin case since it requires few assumptions about the form of the dependence of final parameters on initial parameters and has so far predicted remnant parameters with very small residual error.

So far, fitting of the recoil of the remnant has not been investigated. In order to perform this fit for the SXS catalogs, it will be necessary to compute the remnant momentum from the spherical harmonic decomposition of the gravitational wave strain. A python script to do this exists in the SpEC codebase.

In order to compare the fitting methods used here to those of previous work, it will be necessary to integrate code for previous fits with analysis code for this project. Ref. [4] has code available, and Ref. [8] has explicit formulas and tables of parameters obtained by least-squares fits. A goal will be to finish implementing the fitting formulas in Ref. [8] and to incorporate the Ref. [4] code into the analysis and plotting scripts for this work to compare gaussian process regression fits to previous fits.

REFERENCES

[1] B. P. Abbott *et al.* (LIGO Scientific Collaboration, Virgo Collaboration), Phys. Rev. Lett. **116**, 061102 (2016), arXiv:1602.03837 [gr-qc].
[2] Y. Pan, A. Buonanno, A. Taracchini, L. E. Kidder, A. H. Mroué, H. P. Pfeiffer, M. A. Scheel, and B. Szilágyi, Phys. Rev. D **89**, 084006 (2013), arXiv:1307.6232 [gr-qc].
[3] J. Healy, C. O. Lousto, and Y. Zlochower, Phys. Rev. D **89**, 104052 (2014), arXiv:1406.7295 [gr-qc].
[4] X. Jiménez-Forteza, D. Keitel, S. Husa, M. Hannam, S. Khan, and M. Pürrer, Phys. Rev. **D95**, 064024 (2017), arXiv:1611.00332 [gr-qc].
[5] C. O. Lousto, M. Campanelli, and Y. Zlochower, Class. Quantum Grav. **27**, 114006 (2010), arXiv:0904.3541 [gr-qc].
[6] Y. Zlochower and C. O. Lousto, Phys. Rev. D **92**, 024022 (2015).
[7] http://www.black-holes.org/waveforms.
[8] J. Healy and C. O. Lousto, Phys. Rev. **D95**, 024037 (2017), arXiv:1610.09713 [gr-qc].