Determining remnant parameters from black-hole binary systems Interim Report 2 (revised) - LIGO Document T1700339

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Computing the remnant mass, spin, and recoil of a black hole binary in principle requires numerical relativity (NR) simulations. Unfortunately, NR simulations cannot be performed quickly enough for some waveform models and LIGO data analysis routines that require remnant parameters. We develop phenomenological formulae for the remnant mass, spin, and recoil of binary systems given arbitrary initial spins and mass ratios. We do this by constructing fits to NR simulations in the SXS catalog. In particular, we explore the use of gaussian process regression. We use the SXS catalog to compare the accuracy of our remnant mass and spin fits with that of the remnant mass and spin formulae in the Effective One Body (EOB) waveform model in the LSC Algorithm Library (LALSuite).

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 information about the observable universe.

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. Approximate formulas for these final parameters 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. We also hope to explore whether it is advantageous to use 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 Gaussian Process Regression for remnant parameter fits.

It will be important to compute the error of the new fits constructed here. The reduction of this error compared to the results of previous studies 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.

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 and spin for the case where the initial black holes have zero spin and we found good agreement between the data and the model (see Figures 1, 2, 3). Next, we treat the case where the black holes have spins aligned or anti-aligned with the orbital angular momentum and compare this with [8]; residual plots are given in Figures 4 and 5. The remnant mass for generic spins is then fit with results summarized in Figure 6 and Table I. Work for the remainder of the project will focus on fitting remnant spin in the arbitrary spin case, followed by fitting of recoil in the aligned and arbitrary spin case.

Gaussian Process Regression

A Gaussian Process can be viewed as a means of applying a nonlinear transformation to training data, and then linearly combining the results to predict the value of a function at a new input point [9]. This nonlinear transformation is given by a "kernel" function defined between two input points, which is often a squared-exponential or "radial basis function" (RBF) [9]. Parameters of this

function are referred to as "hyperparameters". In contrast to a parametric fit, which optimizes parameters of a given function according to training data, Gaussian Process Regression optimizes kernel hyperparameters, so that the trained model uses the training data itself to predict function values at new points [9].

The Gaussian Process Regression class provided by `sklearn` is used to perform the fits. This package provides a procedure to train a Gaussian Process model in which kernel hyperparameters are determined by maximizing log-marginal-likelihood [10]. Unless otherwise noted, the default RBF kernel is used.

Training / Validation Partitioning and Cross Validation Routine

In order to accurately estimate fitting error, a validation set is separated from remaining data and excluded from the fit; a model's ability to predict correct values for the validation set is used as a proxy for its error in general. The histograms in Figures 4, 5, 6 report residuals for both the training and validation subsets of data.

In addition, a 10-fold cross validation routine was developed using the `KFold` class in `sklearn.model_selection`. In this procedure, the data is shuffled and then partitioned into ten equal blocks. For each of these blocks, a fit is performed on the other nine blocks and then evaluated on the block not used in fitting. Table I contains norms produced by the cross validation procedure for the Gaussian Process Regression fit to the remnant mass of the generic spin case, when setting the noise parameter "alpha" [10] to 10^{-4}.

Fitting residuals

Zero initial spin

Gaussian Process Regression was used to fit the final remnant mass and spin magnitude in the case of initial spins with a squared magnitude of less than 10^{-10}. Forty-eight points meeting this criterion were used in the fits.

From the residuals in Figure 2 it can be seen that the error in the fit is within 0.1% for all simulations. In the top plot in Figure 1 the best value fit appears smooth and appears to interpolate well for input mass ratios between 1 and 10. Plots for the remnant spin and residuals in the initially spinless case appear in Figures 1 (bottom) and 3.

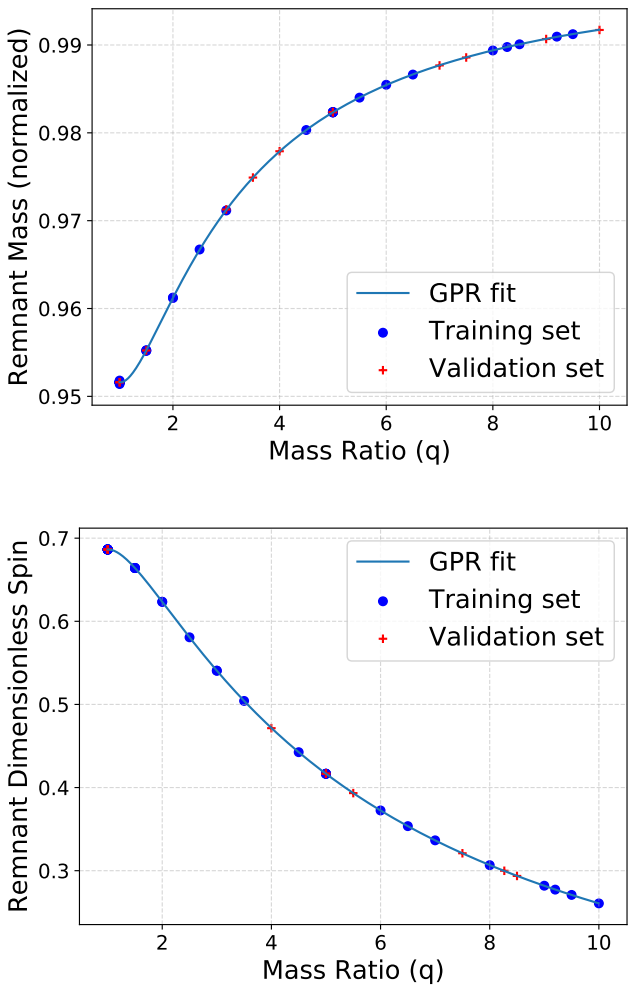
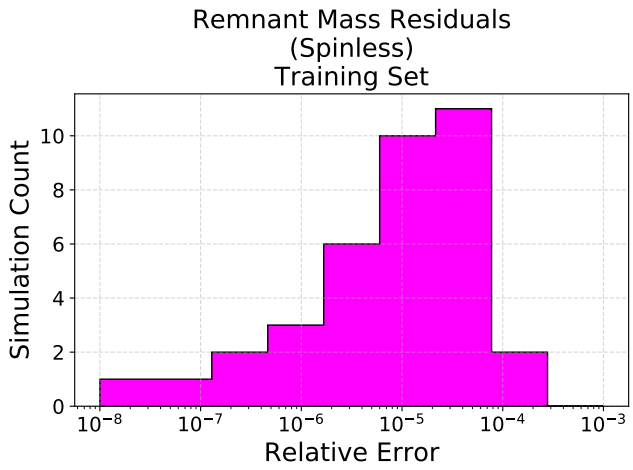


FIG. 1. Plot of predicted remnant mass (solid curve, top) and predicted remnant spin (solid curve, bottom) for spinless case from Gaussian Process Regression fit, each with training data set (solid dots) and validation set (plus signs) overlayed. The training set was used to fit the Gaussian Process 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). 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.

Aligned / anti-aligned initial spin

The validation residuals obtained from the Gaussian Process Regression fit for remnant mass and spin magnitude on the SXS catalog aligned spin data improved on residuals produced by the remnant mass formula in Ref. [8] using the published coefficients (see Figure 4 - the Gaussian Process Regression fit errors are clustered closer to zero in both the training and validation sets). Additionally, a least-squares fit of the remnant mass formula in Ref. [8] was performed on the SXS catalog aligned spin data, and the Gaussian Process fit performed better



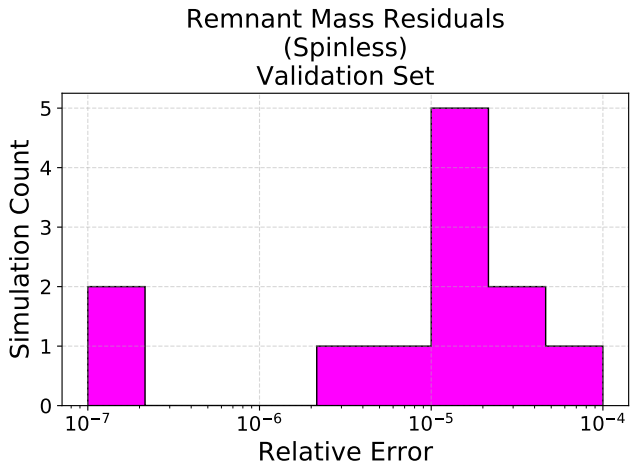
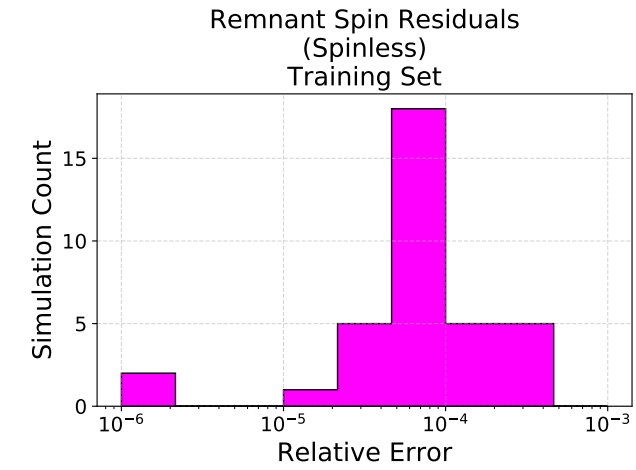


FIG. 2. Training set residuals (top) and validation set residuals (bottom) for a Gaussian Process Regression fit of the remnant mass for the spinless data. Here 36 randomly selected training points were used for the fit out of the 48 spinless simulations, and the remaining 12 formed the validation set. 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.



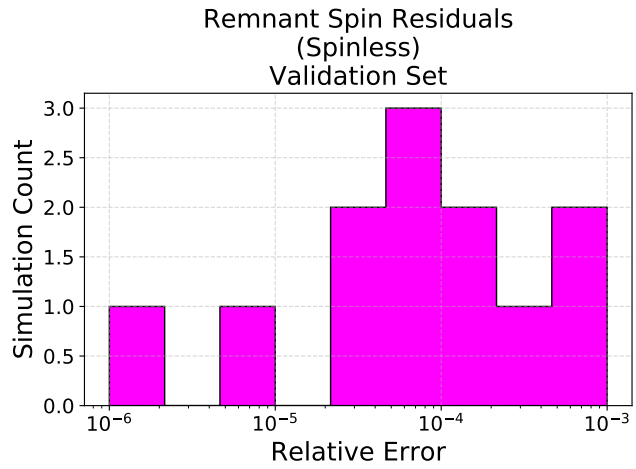


FIG. 3. Training set residuals (top) and validation set residuals (bottom) for a Gaussian Process Regression fit of the remnant spin magnitude for the spinless data.

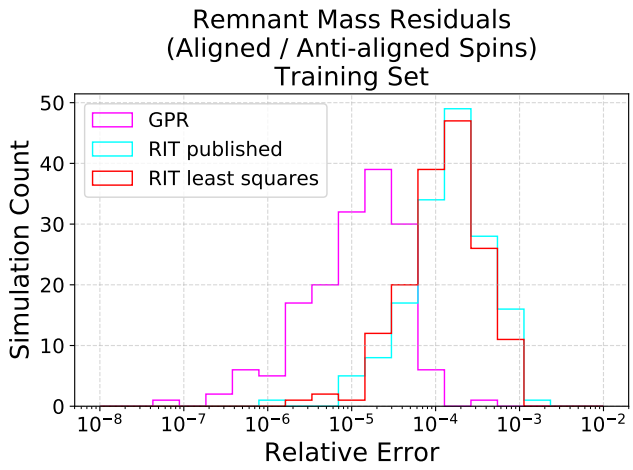
(Figure 4).

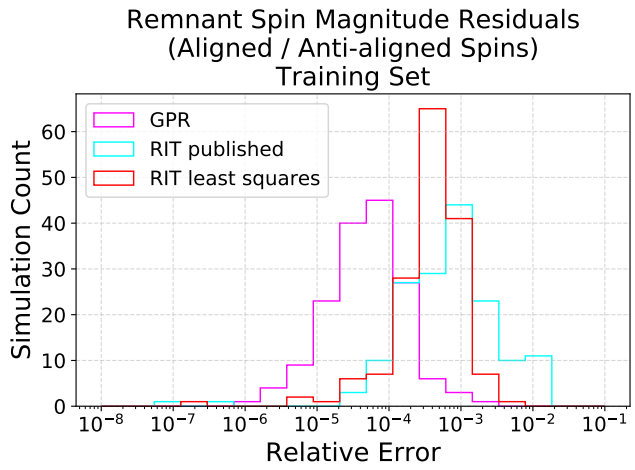
Arbitrary initial spin

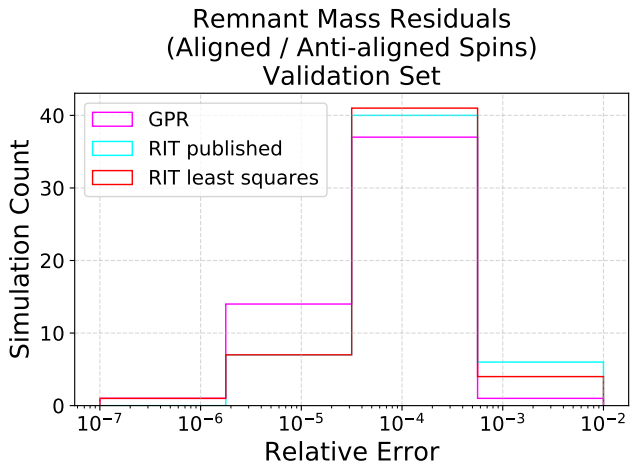
A Gaussian Process Regression fit was performed for the remnant mass in the generic spin case. In Figure 6 and Table I, it can be seen that typical errors are well under 1% and the maximum absolute error is estimated to be of order 1%. Table I summarizes normed quantities from a cross validation analysis of the generic input spin fit.

TABLE I. Relative error norms for the cross validation of the Gaussian Process Regression fit of remnant mass for the arbitrary spin case. Units are in percent or 10^{-2}. The norms are computed for the residual set X as $L_1 = \frac{1}{|X|}\sum_{x\in X}|x|$, $L_2 = \frac{1}{|X|}\sqrt{\sum_{x\in X} x^2}$, $L_{\rm inf} = \max_{x\in X}|x|$. Columns 1-10 represent the partition subset withheld from fitting and used in validation; the mean of each norm is given in the final column.

	Validation Subset										
	1	2	3	4	5	6	7	8	9	10	Mean
L1	0.15	0.11	0.12	0.15	0.11	0.12	0.12	0.12	0.14	0.1	0.12
L2	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02
Linf	1.43	0.84	1.09	1.57	0.76	1.14	0.96	0.85	0.82	1.34	1.08







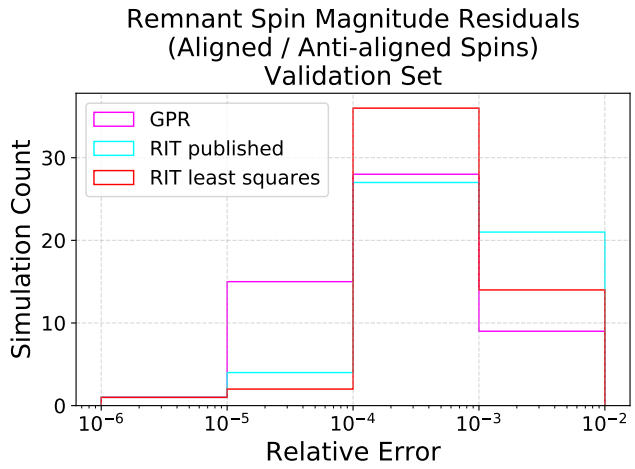


FIG. 4. Training set residuals (top) and validation set residuals (bottom) for Gaussian Process Regression and Ref. [8] fits of the remnant mass in the aligned / anti-aligned input spin case (3 dimensional input parameter space). A total of 212 aligned spin data points were chosen from the public and incoming SXS catalogs by selecting all BBH simulations for which both initial spins retained at least 99.9 percent of their magnitude when the inner product was taken with the initial angular momentum direction; these points were partitioned into a training set and a smaller validation set. "RIT published" refers to residuals obtained using the remnant mass model in Ref. [8] with the published coefficients. "RIT least squares" refers to the same model using coefficients determined by a least squares fit against the training set. Fitting was performed on the relaxed input parameters (parameters measured after the dissipation of junk radiation). 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.

FIG. 5. Training set residuals (top) and validation set residuals (bottom) for a Gaussian Process fit of the remnant spin in the aligned / anti-aligned input spin case.

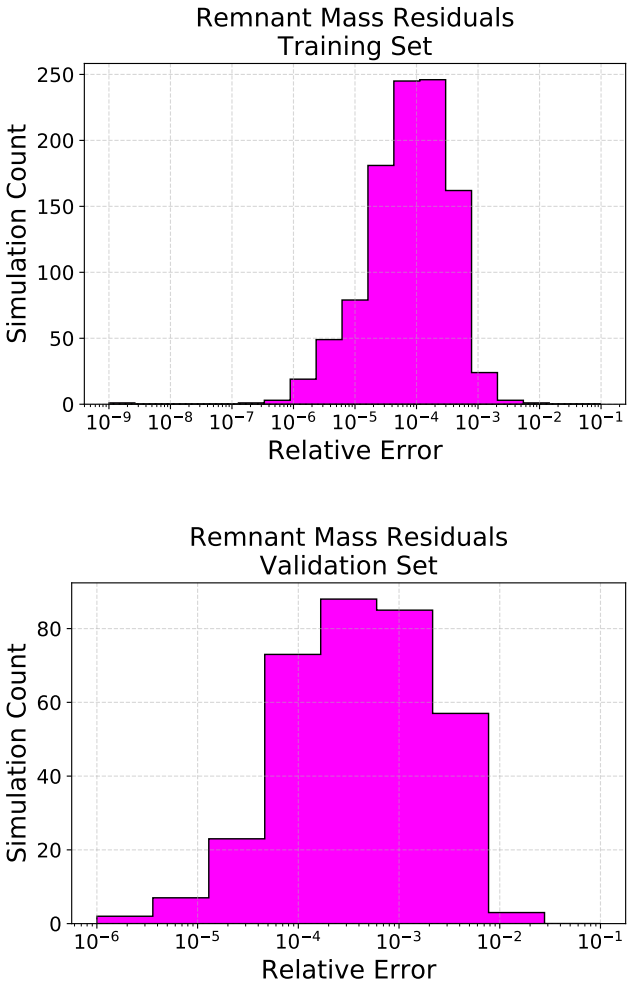


FIG. 6. Training set residuals (top) and validation set residuals (bottom) for a Gaussian Process fit of the remnant spin in the arbitrary spin case (7 dimensional input space). The training and validation sets were partitioned from 1352 black hole binary simulations with arbitrary initial spins.

TABLE II. Relative error norms of remnant mass predictions on the SXS catalog data from models currently used in LALSimulation. Units are in percent or 10^{-2}. The L_1, L_2, and $L_{\rm inf}$ norms are defined as in Table I

	L_1	L_2	$L_{\rm inf}$
EOBNR	0.85	0.03	7.76
EOBNRv2	0.78	0.03	7.44
EOBNRv2HM	0.78	0.03	7.44
SEOBNRv1	0.45	0.02	4.48
SEOBNRv2	0.14	0.01	0.93
SEOBNRv4	0.14	0.01	0.93

Comparison to SEOBNRv4 in LALSimulation

The implementation of the SEOBNRv4 model in `src/LALSimBlackHoleRingdown.c` was used to predict remnant parameters for the SXS catalog data. The source code was minimally modified and incorporated into fitting python scripts using `ctypes`.

Table II summarizes the normed residuals for the models currently implemented in LALSimulation when applied to the SXS catalog data. In Table I, the mean maximum absolute relative error is 1.08% for the Gaussian Process Regression mass fit, which is slightly higher than the $L_{\rm inf}$ of 0.93% for SEOBNRv2 and SEOBNRv4. Conversely, the average absolute relative error is improved in the Gaussian Process Regression fit from 0.14% to 0.12%.

CHALLENGES

Uncertainties in recoil computations

Although the output of the code includes the final coordinate velocity of the remnant, this is only a coordinate velocity and not physically meaningful. Much better is to compute recoils from the gravitational waveform; in our case we use the spherical harmonic decomposition of the Weyl scalar Ψ_4 [11]. This is currently implemented in a script in SpEC.

So far, the magnitude of the radiated linear momentum calculated by this procedure has varied by up to order 10% or higher between resolution levels in the same simulation, even for cases with high recoil. For comparison, initial and remnant mass and spin typically vary by less than 0.1% between resolution levels for the same data set. The problem was initially worse due to contributions from "junk radiation" (gravitational radiation produced by artifacts of the simulation itself) at early times. Although integrating starting at a time after the dissipation of the junk radiation has improved results, the aforementioned discrepancies still exist. It will be important to establish the extent to which the differences are due to expected numerical uncertainties, and whether there are any mistakes in the current data treatment.

Parameter choices in full dimensional spin and recoil fits

Although good residuals have been obtained for remnant mass in the full dimensional case, it may be more difficult to fit the remnant spin. This is primarily due to the fact that input and output parameters must be chosen carefully; it is possible that the current Cartesian representation of the spins will not work well for fitting. Although there is no information difference between different coordinate representations of the spins, these choices may be significant in fitting; for example, in the spinless case it was observed that directly using the mass ratio q or not normalizing masses by the total initial mass in fitting yielded errors which were higher by several orders of magnitude[1]. Using the larger normalized mass[2] as the input parameter and using the normalized remnant mass as the output parameter yielded the results shown in Figures 1, 2, and 3.

Fitting the recoil will similarly require well chosen parameters, and in addition is expected to have much higher uncertainties than the other quantities. Because large numbers of the simulations are not expected to have recoil, and indeed currently have a computed recoil which appears to be numerical noise, it will be important to account for this to avoid overfitting and when measuring relative error.

GOALS

The first priority will be implementing fits to spin in the general initial spin case. After this, the current values for recoil will be revisited and recomputed if any errors are found in how they were computed. Once this is done, and appropriate uncertainty is determined for the recoil of each simulation, fits to the recoil will be performed.

A thorough comparison between the Gaussian Process fits and the EOB waveform models implemented in LAL-

[1] The two suboptimal choices of parameters reflect two separate issues: fitting from the mass ratio q did not work well because Gaussian Process Regression fits seem to perform better when the input parameters are normalized; fitting using non-normalized masses did not work well because a relatively small number of early simulations did not normalize all masses by the initial mass [12]. Because Gaussian Process Regression uses locality to predict function values at new points, error can be higher when predicting a function at points far away from the training set points. Because remnant mass scales linearly with initial mass, failing to normalize masses by the initial mass causes artificially large distances between some data points.

[2] Here, the larger normalized mass refers to the quantity $q/(q+1)$, where q is the ratio of the larger mass to the smaller mass.

Suite will be performed as well, and work on this will proceed throughout the remainder of the project.

ACKNOWLEDGMENTS

Fits and analysis were performed on the wheeler machine. The SXS simulation catalog provided data for fitting. The NSF, the LIGO lab, and SFP at Caltech provided funding and resources for the project. Fitting procedures and analysis used the `sklearn` package. Code from LALSimulation in LALSuite was incorporated into analysis routines for comparison.

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