Abstract

We consider two example systems, a logistic-growth population model and a damped spring-mass model. These models are each parameterized in two different ways. In one case (the logistic) the parameters are independent in one formulation and dependent in the other. In the other example (the spring-mass), the parameterizations are each independent. We carry out a series of inverse problems for these examples using ordinary least squares on each model. We use uncertainty quantification methods involving asymptotic theory to investigate for evidence of parameter dependence. We examine the off-diagonal elements of the Fisher Information (covariance) matrix to compare the matrices created by dependent and independent parametrizations. We further compare the use of exact vs. asymptotic confidence ellipsoids. Finally we compare the confidence ellipsoids generated by asymptotic theory to those created using Monte Carlo simulations.

Key Words: Inverse problems, effects of parameterizations, independent vs. dependent, exact vs. asymptotic confidence ellipsoids, Monte Carlo simulations.
1 Introduction

Given a data set from some particular system under study, scientists often attempt to model this system mathematically. This typically leads to an inverse problem, in which a mathematical model is fit to a given data set in order to validate the model and subsequently make observations and predictions about the real system.

For any mathematical model, there are typically several different yet equivalent formulations in the sense that different parameters are used in the mathematical model, but the overall formulations are all capable of describing the data in the exact same manner. While it may seem intuitive that all of these formulations should thus perform equivalently in describing data through an inverse problem, the dependence of different parameterizations in a particular model may influence how well it can describe a certain data set. The relationship between parametrizations can be examined using tools arising naturally from a process known as uncertainty quantification. There are several types of uncertainty quantification that can be used to determine reliability information about parameters including asymptotic theory, bootstrapping, Monte Carlo simulations and Bayesian techniques. Asymptotic theory is not computationally time consuming, and produces the least amount of information about parameters estimated through an inverse problem. Bootstrapping and Monte Carlo simulation are more computationally intensive and subsequently creates more information, while Bayesian is generally the most time-consuming of the methods. The main goal of this project is one of studying the nature of parametrizations: we seek to determine whether or not it is possible to detect indications of parameter dependence in asymptotic theory, thereby minimizing computational time that is usually associated with determining this information. In this note, we investigate the parametrization process on two distinct mathematical models. For each mathematical model, we will estimate the correlation of estimators in a given parametrization by computing covariance matrices numerically. We are expecting to see a higher correlation in some parametrizations than others due to the different equations that generate them, and this correlation might be evidenced by non-trivial off-diagonal entries of the covariance matrix. We also use confidence ellipsoids in our analyses. We will also compute parameter distributions for each model and several parameter sets in order to effectively compare the results of Monte Carlo simulation and asymptotic theory, as the parameter distributions might be a more reliable indicator of the relationship between parameters.

To analyze the effects of the different parametrizations on the inverse problem, we will compute 2-dimensional confidence ellipsoids. Smaller and flatter confidence ellipsoids should suggest that we are able to estimate the true parameter for a given data set with more confidence. In this analysis, we will also be using two different types of confidence ellipsoids, an asymptotic confidence ellipsoid (based on a fundamental linearization-see [9]) and an exact confidence ellipsoid to test the effects of linearity on confidence ellipsoid computations. We then use Monte Carlo simulations to compare the resulting “ellipsoids” to those obtained using asymptotic theory.

The two models under consideration are the spring oscillator system and the logistic growth model, which are both very commonly used and important, mathematical models in numerous areas of science.

2 Mathematical model descriptions

2.1 Spring equation

The first model we consider is the spring-mass-dashpot system with mass $m$, damping coefficient $c$, and spring constant $k$. If $C = c/m$ and $K = k/m$, then the oscillating spring (in a standard engineering and mathematical formulation) may be modeled as (we shall refer to this as independent parametrization 1)

$$\frac{d^2y(t)}{dt^2} + C\frac{dy(t)}{dt} + Ky(t) = 0,$$

$y(t_0) = y_0, \quad \dot{y}(t_0) = v_0.$

In this project, we take $y(t_0) = \frac{1}{2}$ and $\dot{y}(t_0) = 0$ for noise levels and parameter sets.

Because Equation (1) is a homogeneous second order differential equation, we can solve it analytically. This analytic solution will have the form
\[ y(t) = e^{-\frac{C}{2}t}(A \cos(\omega t) + B \sin(\omega t)), \quad (2) \]

which can be further modified [7] to

\[ y(t) = e^{-\frac{C}{2}t}(R \sin(\omega t + \delta)), \quad (3) \]

where \( \delta \) (or \( A \) and \( B \)) can be determined from the initial conditions. The solution will be bounded by the damping envelope, \( Re^{-\frac{C}{2}t} \),

\[ |y(t)| \leq Re^{-\frac{C}{2}t}. \]

By solving the characteristic polynomial of Equation (1), we find that

\[ \omega = \sqrt{\frac{4K - C^2}{2}}, \quad (4) \]

or that, equivalently,

\[ K = \omega^2 + \frac{C^2}{4}. \quad (5) \]

And thus we can reformulate Equation (1) to the form

\[
\frac{d^2y(t)}{dt^2} + C\frac{dy(t)}{dt} + \left( \omega^2 + \frac{C^2}{4} \right) y(t) = 0. \quad (6)
\]

Note that this also provides a 2-parameter \((\omega, C)\) independent parametrization (called independent parametrization 2 below) of the damped spring-mass equation.

Throughout this presentation, we will examine two different parameter sets of this spring oscillator system by adding various noise levels, \( nl \), that have been sampled from a normal distribution with mean 0 and standard deviation \( \sqrt{nl} \). The parameter values used for each data set are given in Table 1, and each system is plotted with no noise \((nl = 0)\) in Figure 1. These parameter sets will be denoted by their corresponding number in the left hand column of Table 1.

<table>
<thead>
<tr>
<th>Parameter set</th>
<th>( C )</th>
<th>( K )</th>
<th>( \omega )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1/2</td>
<td>1/2</td>
</tr>
<tr>
<td>2</td>
<td>1/3</td>
<td>1/9</td>
<td>1/(2\sqrt{3})</td>
</tr>
</tbody>
</table>

Table 1: Description of different parameter sets under consideration.

### 2.2 Logistic Model

The second model we consider is the widely used mathematical model for a bounded, dynamic population is the logistic model, given by the differential equation

\[ \dot{P}(t) = rP(t) \left( 1 - \frac{P(t)}{K} \right), \quad (7) \]

where \( r \) is the intrinsic growth rate, and \( K \) is the carrying capacity for the population under consideration. By distributing the intrinsic growth rate and carrying capacity over the \( P(t) \), we may modify Equation (7) to obtain

\[ \dot{P}(t) = AP(t) - BP(t)^2. \quad (8) \]
Figure 1: Plots of forward solutions corresponding to the parameter sets 1 and 2 under consideration for the spring oscillator system with no noise added.

Note that if we set $A = r$ and $B = K$ we see that the models are equivalent but the parameters are not independent in the second formulation (8).

We will again consider two different parameter sets (denoted by parameter sets 1 and 2 below) for the logistic model. These parameter sets are given in Table 2. The forward solutions for these parameter sets are also plotted with no noise in Figure 2.

<table>
<thead>
<tr>
<th>Parameter set</th>
<th>$r (=A)$</th>
<th>$K$</th>
<th>$B$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$1/2$</td>
<td>8</td>
<td>$1/16$</td>
</tr>
<tr>
<td>2</td>
<td>$1$</td>
<td>5</td>
<td>$1/5$</td>
</tr>
</tbody>
</table>

Table 2: Description of different parameter sets for the logistic model under consideration.

3 Methodology

3.1 Statistical Analysis and Covariance Matrices

For our parameter estimation methodology, we will consider a scalar mathematical model of the form

$$\frac{dy(t)}{dt} = g(t, y(t), \hat{\theta}),$$  \hspace{1cm} (9)

which is representative of the spring or logistic differential equations, $t$ is time, $y(t)$ are the model solutions at that time, and $\hat{\theta}$ is the parameter vector. We will assume a constant variance statistical model for our data of form

$$Y_j = f(t_j, \bar{\theta}_0) + \varepsilon_j, \hspace{0.5cm} j = 0, 1, ..., n$$ \hspace{1cm} (10)

where $Y_j$ represents the $j^{th}$ data point with realizations $y_{data,j}$, $f(t_j, \bar{\theta}_0)$ is the forward mathematical model solution for our truth parameter $\bar{\theta}_0$, and the $\varepsilon_j$ terms represent the random noise that causes the data to deviate from the true solution. These noise terms may be caused by various sources such as experimental and measurement error. The three noise levels we will be using in this project are 0.01, 0.05, and 0.2. The goal in parameter estimation is to estimate $\bar{\theta}_0$ (which is known to us in our examples) by creating a random variable estimator $\hat{\Theta}$.
whose realizations for a given a set of data are called estimates denoted by \( \hat{\theta} \). This \( \hat{\theta} \) is determined by solving an inverse problem on the created sets of simulated data.

Using the constant variance assumption on our data of Equation (10), we may implement an ordinary least squares formulation, in which we estimate the parameter vector \( \vec{\theta}_0 \), by

\[
\vec{\theta}_0 \approx \hat{\theta} = \arg \min_{\vec{\theta} \in Q} \sum_{j=1}^{n} |y_{\text{data},j} - y(t_j, \vec{\theta})|^2, \tag{11}
\]

where \( y(t_j, \vec{\theta}) \) is the mathematical model solution for a given parameter, \( \vec{\theta} \), and \( Q \) is the set of admissible parameters for \( \vec{\theta} \). We thus define the corresponding cost functional

\[
J(\vec{\theta}) = \sum_{j=1}^{n} |y_{\text{data},j} - y(t_j, \vec{\theta})|^2. \tag{12}
\]

We note that the above equations involve the unknown (and to be estimated) parameters \( \vec{\theta} \) and hence one needs to employ an ordinary least squares algorithm using the above cost functional. All inverse problems were performed in MATLAB using the *lsqnonlin* function and a conventional ordinary least squares iterative procedure. It is important to note that *lsqnonlin* simply takes in the residuals (not the sum of the residuals squared, as seen in the above cost functional), and this was taken into account when performing inverse problems. Although we do not know the probability distribution for our random variable, \( \vec{\theta} \), we can approximate it under asymptotic theory (as \( n \to \infty \)) with a multivariate Gaussian distribution \([9]\) as

\[
\vec{\theta} \sim \mathcal{N}_p(\vec{\theta}_0, \sigma_0^2[\chi^T(\vec{\theta}_0)\chi(\vec{\theta}_0)]^{-1}), \tag{13}
\]

where \( \sigma_0^2 \) denotes the standard deviation and is approximated by the unbiased estimate

\[
\hat{\sigma}^2 = \frac{1}{n - p} \sum_{j=1}^{n} [y_{\text{data},j} - f(t_j, \vec{\theta})]^2. \tag{14}
\]

Here \( p \) denotes the number of parameters being estimated and \( \chi^n \) denotes the sensitivity matrix, given by

\[
\chi_{jk}^n(\vec{\theta}) = \frac{\partial f(t_j, \vec{\theta})}{\partial \theta_k}, \quad j = 0, 1, \ldots, n, \quad k = 1, \ldots, p, \tag{15}
\]
where $\theta_k$ is the $k^{th}$ element of $\tilde{\theta}$. In order to quantify uncertainty in estimating a parameter vector $\hat{\theta} = [\hat{\theta}_1, \hat{\theta}_2]$ for the differential equation in each of our models, covariance matrices, as well as standard errors, can be computed using standard asymptotic theory (as $n \to \infty$).

To determine the entries in the sensitivity matrix, $\chi$, we can solve the differential equation at $\hat{\theta}$

$$\frac{d}{dt} \left( \frac{\partial f}{\partial \theta} \right) = \frac{\partial g}{\partial f} \frac{\partial f}{\partial \theta} + \frac{\partial g}{\partial \theta}. \quad (16)$$

Note that $\frac{dy}{dt} = g(t, y(t), \tilde{\theta})$ is the differential equation being solved and $f(t_j, \tilde{\theta})$ is the forward solution of each model. Because we know the formulas for $\frac{dy}{dt} = g(t, y(t), \tilde{\theta})$, we can solve for Equation (16) by setting up the differential equation in terms of the sensitivity $[3]$.

The $\chi^n$ matrix provides a measure for how sensitive the mathematical model is to its own parameters. This can be used to estimate the $p \times p$ covariance matrix, $\Sigma^0_n$,

$$\Sigma^0_n \approx \hat{\Sigma} = \hat{\sigma}^2 [\chi^n(\hat{\theta})\chi^n(\hat{\theta})]^{-1}. \quad (17)$$

From this, we consider the off-diagonal elements to determine if they are statistically trivial when compared to the diagonal elements of the covariance matrix. Trivial entries will be indicative of independence, while non-trivial entries will suggest that the parameters are correlated.

### 3.2 Confidence ellipsoids

The covariance matrices are a measure to estimate the correlation and standard deviation of the certain estimators of a mathematical formulation but do not provide any information on parameter distribution. Hence there is still more to be shown for demonstrating the relative confidence in parameter estimation for different parameterizations. Here we implement 2-dimensional confidence ellipsoids for our two different models. In each case, we create an ellipse around our $\theta$ estimate that we are $(1 - \alpha)100\%$ confident will contain with $95\%$ confidence ($\alpha = 0.05$) our truth vector, $\hat{\theta}_0$. We also look at $\alpha = 0.1$ and $\alpha = 0.01$. In the following sections we will outline the construction of two different types of confidence ellipsoids: asymptotic confidence ellipsoids and exact confidence ellipsoids. The two confidence ellipsoids are asymptotically equivalent as $n \to \infty$, where $n$ is the number of observations, but the exact confidence ellipsoid should be a bit more precise as it excludes the linearization that is present in asymptotic confidence ellipsoids and it’s formulation does not require the sensitivity matrix $\chi$. The asymptotic confidence ellipsoids do require computing $\chi = \chi^n$, and hence are intuitive when also computing the covariance matrices described above.

For the different formulations of the same mathematical model, the exact same data realizations will be used for consistency and are computed simultaneously with the covariance matrices.

### 3.3 Asymptotic confidence ellipsoids

For the asymptotic confidence ellipsoids, recall that $[3, 5]$ (in abuses of notation below, we drop the superscripts $n$ on $\chi$, $\tilde{\Theta}$, and $J$) :

- $\tilde{\Theta} \sim N(\hat{\theta}_0, \sigma^2(\chi^T \chi)^{-1})$
- The quantity $J(\tilde{\Theta})/(n - p)$ is an unbiased estimator for $\sigma^2$.

and observe that $[5]$:

- $Q_1 = J(\tilde{\Theta})/\sigma^2 \sim \chi^2_{n-p}$, a Chi-square distribution with $n - p$ degrees of freedom.

Define the quantity

$$Q_2 = (\tilde{\Theta} - \hat{\theta}_0)^T \chi^T \chi (\tilde{\Theta} - \hat{\theta}_0)/\sigma^2.\,$$

It can be shown $[8, \text{Thm. 2.9}]$ that $Q_2 \sim \chi^2_p$.
We define
\[ F(\tilde{\Theta}) = \frac{(\tilde{\Theta} - \tilde{\theta}_0)^T \chi T \chi (\tilde{\Theta} - \tilde{\theta}_0)}{ps^2} \] (18)
where \( s^2 = J(\tilde{\Theta})/(n - p) \). Then
\[
F(\tilde{\Theta}) = \left( \frac{(\tilde{\Theta} - \tilde{\theta}_0)^T \chi T \chi (\tilde{\Theta} - \tilde{\theta}_0)}{J(\tilde{\Theta})} \right) \left( \frac{n - p}{p} \right) \left( \frac{\sigma^2}{\sigma^2} \right) = \frac{Q_2/p}{Q_1/(n - p)}.
\]

In both the numerator and denominator we have a Chi-squared distribution which is scaled by its number of degrees of freedom. This is, by definition, the F-distribution. Thus
\[ F(\tilde{\Theta}) = \left( \frac{(\tilde{\Theta} - \tilde{\theta}_0)^T \chi T \chi (\tilde{\Theta} - \tilde{\theta}_0)}{J(\tilde{\Theta})} \right) \left( \frac{n - p}{p} \right) \left( \frac{\sigma^2}{\sigma^2} \right) = Q_2/p \frac{Q_1}{Q_1/(n - p)}.
\]

It follows that an approximate \((1 - \alpha)\) confidence interval is [2, 5]:
\[
\{ \tilde{\Theta} : (\tilde{\Theta} - \hat{\Theta})^T \chi T \chi (\tilde{\Theta} - \hat{\Theta}) \leq ps^2 F_{p,n-p}^\alpha \}
\] (20)
where \( F_{p,n-p}^\alpha \) is the upper-\( \alpha \) critical value of the \( F_{p,n-p} \) distribution and \( \hat{\Theta} \) is the parameter estimated by the inverse problem. This is the asymptotic confidence ellipsoid for the OLS estimate \( \hat{\Theta} \).

### 3.4 Exact confidence ellipsoids

For exact confidence ellipsoids, consider the least squares equation :
\[ J(\tilde{\Theta}) = \| \tilde{Y} - f(\tilde{\Theta}) \|^2 \] (21)
We saw that (19) is an approximate \( 100(1 - \alpha)\% \) confidence region for \( \Theta \). For varying \( \alpha \) the regions are enclosed by ellipsoids which are also contours of the approximate multivariate normal density function of \( \tilde{\Theta} \). Since \( J(\tilde{\Theta}) \) measures the "closeness" of the observations to the fitted equation for any \( \tilde{\Theta} \), we can base confidence regions for \( \tilde{\Theta} \) on the contours of \( J(\tilde{\Theta}) \) [9]. This takes the form of:
\[
\{ \tilde{\Theta} : J(\tilde{\Theta}) \leq cJ(\hat{\Theta}) \}
\] (22)
where \( c > 1 \). These are exact confidence regions. Now the task is to find an appropriate value of \( c \). According to [9], we have this approximation:
\[ J(\tilde{\Theta}) - J(\hat{\Theta}) \approx (\tilde{\Theta} - \hat{\Theta})^T \chi T \chi (\tilde{\Theta} - \hat{\Theta}). \] (23)
Therefore, since
\[
(\tilde{\Theta} - \hat{\Theta})^T \chi T \chi (\tilde{\Theta} - \hat{\Theta}) \leq ps^2 F_{p,n-p}^\alpha,
\] (24)
as shown in the asymptotic confidence section, we can then establish the inequality:
\[ J(\tilde{\Theta}) - J(\hat{\Theta}) \leq ps^2 F_{p,n-p}^\alpha, \] (25)
where \( F_{p,n-p}^\alpha \) is the upper-\( \alpha \) critical value of the \( F_{p,n-p} \) distribution. From [9], we have that
\[ s^2 = \frac{J(\tilde{\theta}_0)}{n - p}, \] (26)
where $s^2$ is a completely independent estimate of the variance $\sigma^2$. Now we can substitute (26) into (25):

$$J(\tilde{\theta}) - J(\hat{\theta}) \leq J(\hat{\theta}) \frac{p}{n-p} F_{p,n-p}^\alpha.$$

(27)

And finally, we rearrange (27) to get:

$$\{ \tilde{\theta} : J(\tilde{\theta}) \leq J(\hat{\theta})(1 + \frac{p}{n-p} F_{p,n-p}^\alpha) \}$$

(28)

which is the exact confidence ellipsoid described in (22), and $c = 1 + \frac{p}{n-p} F_{p,n-p}^\alpha$. Thus, (28) will have the required asymptotic confidence level of $100(1 - \alpha)$%. This is the exact confidence ellipsoid for the OLS estimate. For finite $n$, the exact and approximate confidence regions can be very different, which could indicate the inadequacy of linear approximations in asymptotic intervals. Exact ellipsoids are more difficult to compute and display; however, they might be more likely to provide accurate estimation of the real confidence ellipsoid.

3.5 Parameter distributions via Monte Carlo simulations

Parameter distributions were created in this study as another way for assessing parameter dependence in a model. To implement this technique as a way of quantifying uncertainty in the parameter estimates for both logistic and spring models, we first obtained a vector of true parameters from the parameter sets for each model, $\theta_0$, and ran a forward solution of each model to obtain data. To make this more realistic, we then created noise using three different levels of 0.01, 0.02, and 0.05. The forward solution was modified by then randomly adding or subtracting a number between zero and one of the three noise levels. This way, we were able to create 1000 simulated data sets for each parameter set and each noise level which can then be solved using the inverse problem methodology described in Section 3.1. Thus for each parameter set and each noise level, we obtain 1000 estimated parameters $\hat{\theta}$. These are then plotted to create a parameter distribution, in which we are looking for randomness. Any form of a pattern is indicative of dependence and correlation between the estimated parameters. Independence between parameters will result in a random scattering of parameter values.

4 Motivation

From the above sections outlining different formulations of equivalent mathematical models, one may initially believe that both formulations should be equally effective in estimating parameters for a given set of data. This may not be the case, however, as the change of variables creates different parameter spaces for all of the estimators in the mathematical models. This information is more clearly established in the Bayesian method of uncertainty quantification.

From the previous sections, we see that these reparameterizations will establish different probability density functions for each of the estimators. Although we do not know the actual probability density functions, we can approximate them under asymptotic theory [1] and we can simulate the probability distribution through Monte Carlo simulation results. In order to investigate these probability density functions (and hence how confidently we can estimate these parameters through an inverse problem), we will compute confidence ellipsoids for different levels of noise for each parameter set for each mathematical model. We hope that using the off-diagonal elements of the covariance matrix to detect correlation between parameters for a parameter set might give us a hint of what to expect in the confidence ellipsoids' relative angle and size. For this reason, we have computed the covariance matrices for each formulation of both math models slightly before constructing our confidence ellipsoids. We will later on use these to see if we have a noticeable connection between correlation magnitude and confidence ellipsoid size.

5 Covariance matrix results

Here we have computed covariance matrices for two formulations for both of our mathematical models. All will be $2 \times 2$ matrices where the diagonal elements will estimate the standard error associated for the corresponding
Table 3: Covariance matrices for the spring oscillator system and parameters: $C = 1$, $K = 1/2$ or $C = 1$, $\omega = 1/2$.

<table>
<thead>
<tr>
<th>noise</th>
<th>C, K</th>
<th>C, K</th>
<th>C, K</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01</td>
<td>0.00134, 0.000674</td>
<td>0.00136, 0.000678</td>
<td>0.00121, 0.000605</td>
</tr>
<tr>
<td>0.05</td>
<td>0.00674, 0.00141</td>
<td>0.00678, 0.00142</td>
<td>0.00605, 0.00127</td>
</tr>
<tr>
<td>0.20</td>
<td>0.0365, 0.0180</td>
<td>0.0360, 0.0184</td>
<td>0.0360, 0.0153</td>
</tr>
</tbody>
</table>

parameter estimator and the off diagonal elements will serve as an estimation of the correlation between two separate parameters. Tables 3 - 4 represent parameter sets one and two for the spring model, and each consists of three covariance matrices for each noise level. Tables 5 - 6 for parameter sets one and two, the same is done for the logistic model. In both scenarios, noisy constant variance data was created using Equation (10) for $nl = 0.01$, 0.05, and 0.2. In each case, three separate noisy data sets were created for each noise level and covariance matrices for each data set were calculated for both parameterizations of each model. For example, in Table 3, the first covariance matrix in the $nl = 0.01$ row for C-K and the first covariance matrix in the $nl = 0.01$ row for C-$\omega$ correspond to the same noisy data set for the first spring oscillator parameter set. The matrix in the same position of Table 4 was created using the exact same realization of data.

5.0.1 Spring Oscillator

For the spring oscillator system, it is important to note that for both parameterizations and both parameter sets, the diagonal elements are all of the same magnitude for most of the entries. For parameter set 1, the off-diagonal elements of the C-$\omega$ parametrization are one order of magnitude smaller than those of the C-K parametrization for a noise level of 0.01. For the noise level of 0.05, the off-diagonal entries of the C-$\omega$ are all on the order of $10^{-4}$, while the C-K elements are on the order of $10^{-2}$. For the noise level of 0.2, the off-diagonal elements of the C-$\omega$ parametrization are on the order of $10^{-3}$, while the C-K parametrization has entries on the order of $10^{-1}$. The difference between the two parameterizations is only slightly distinguishable, and we must take into account that the off-diagonal elements for both parameterizations are non-trivial relative to the main diagonal entries. Therefore, since the off-diagonal elements are usually within an order of magnitude of the diagonal entries, we cannot definitively say that any of the off-diagonal elements are actually trivial.

For parameter set 2, the same thing essentially occurs. The main diagonal elements are all relatively similar for both parameterizations and all noise levels. The C-$\omega$ parametrization still has slightly lesser orders of magnitude and are closer to zero. However, the off-diagonal elements are still within an order of magnitude when compared to the diagonal elements in the matrix, and thus we cannot say that off-diagonal elements are actually trivial.

Covariance patterns are the same for each of the two independent parametrizations of the damped spring-mass
<table>
<thead>
<tr>
<th>noise</th>
<th>C</th>
<th>K</th>
<th>C</th>
<th>K</th>
<th>C</th>
<th>K</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01</td>
<td>C 1.261e-05 4.354e-06</td>
<td>C 1.159e-05 3.989e-06</td>
<td>C 1.255e-05 4.301e-06</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>K 4.354e-06 3.696e-05</td>
<td>K 3.989e-06 3.399e-05</td>
<td>K 4.301e-06 3.674e-05</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.05</td>
<td>C 0.000325 0.000113</td>
<td>C 0.000338 0.000116</td>
<td>C 0.000270 9.163e-05</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>K 0.000113 0.000953</td>
<td>K 0.000116 0.000993</td>
<td>K 9.163e-05 0.000793</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.20</td>
<td>C 0.00429 0.00137</td>
<td>C 0.00557 0.00205</td>
<td>C 0.00476 0.00165</td>
<td></td>
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<td></td>
</tr>
<tr>
<td></td>
<td>K 0.00137 0.0124</td>
<td>K 0.00205 0.0164</td>
<td>K 0.00165 0.0139</td>
<td></td>
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<td></td>
</tr>
</tbody>
</table>

Table 4: Covariance matrices for the spring oscillator system and parameters: \( C = \frac{1}{3}, K = \frac{1}{9} \) or \( C = \frac{1}{3}, \omega = \frac{1}{2\sqrt{3}} \).

<table>
<thead>
<tr>
<th>noise</th>
<th>r</th>
<th>K</th>
<th>r</th>
<th>K</th>
<th>r</th>
<th>K</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01</td>
<td>r 7.414e-06 -1.806e-05</td>
<td>r 6.956e-06 -1.729e-05</td>
<td>r 6.675e-06 -1.646e-05</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>K -1.806e-05 0.000564</td>
<td>K -1.729e-05 0.000539</td>
<td>K -1.646e-05 0.000514</td>
<td></td>
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<tr>
<td>0.05</td>
<td>r 0.000199 -0.000492</td>
<td>r 0.000183 -0.000426</td>
<td>r 0.000176 -0.000422</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>K -0.000492 0.0153</td>
<td>K -0.000426 0.0134</td>
<td>K -0.000422 0.0132</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.20</td>
<td>r 0.00313 -0.00822</td>
<td>r 0.00257 -0.00496</td>
<td>r 0.00298 -0.00866</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>K -0.00822 0.253</td>
<td>K -0.00496 0.158</td>
<td>K -0.00866 0.270</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 5: Covariance matrices for the logistic model and parameters: \( r = 1/2, K = 8 \) or \( A = 1/2, B = 1/16 \).
Table 6: Covariance matrices for the logistic model and parameters: \( r = 1, K = 5 \) or \( A = 1, B = 1/5 \).

5.0.2 Logistic Model

For parameter set 1 of the logistic model, the \( A \) and \( B \) parametrization has off-diagonal elements that are one order of magnitude smaller than those of the \( r \) and \( K \) parametrization, but the two parameterizations typically share a very similar magnitude, although not as closely as the spring model. When considering the noise level of 0.2, the two parameterizations have off-diagonal elements of the same magnitude. For parameter set 2 the \( r \) and \( K \) parametrization has virtually the same results as the \( A-B \) parametrization. Thus, it is difficult to determine anything when considering dependence or independence of the parameters. Also, the same problem occurs here as in the spring model above: the off-diagonal elements are not trivial when compared to the main diagonal entries. While some of the off-diagonal entries are small, they are often the same magnitude or one order of magnitude less than the other entries in the matrix, thereby making these elements non-trivial.

It should be mentioned that the selection of data points plays an important role in the inverse problem. It is intuitive that the correlation for \( r \) and \( K \) would be smallest with many data points taken at the carrying capacity, as that should allow us to estimate \( K \) very accurately, regardless of the growth rate used before the carrying capacity is reached. This also is in effect for the spring model, as one can see from the left graph (parameter set 1) of 1 completes one oscillation, while the right graph does not. While data points were taken so that the inverse problem would not become singular, there still may have been features of the data that influenced the outcome of the inverse problem, such as duration of time. However, through some manipulation, we created more covariance matrices using different time points but still not allowing the inverse problem to be singular, and these were not significantly different than the ones presented in this paper. This suggests that the overall correlation may be harder to distinguish between our two different parameterizations for the logistic model using only the covariance matrices.
6 Confidence ellipsoid results

Due to the length of time that it takes to compute confidence ellipsoids, only those for the logistic model are shown. The goal of observing these ellipsoids is to see if they present some inclination that there are some differences between the different formulations of each mathematical model. Second, there are also differences between the exact and asymptotic confidence ellipsoids. Below are the results when comparing the two different parameterizations, (7) and (8) of the logistic model and comparing asymptotic vs. exact ellipsoids.

6.1 A-B vs. r-K parametrizations

Notice there is a significant difference between the angles of the confidence ellipsoids for A-B. This is reflected in Table 6, in which there was always a positive correlation for the $A$ and $B$ parametrization and a negative correlation $r$ and $K$ parametrization. Also, the A-B parametrization produces slightly flatter ellipsoids than the $r$-$K$ parametrization relative to scale. Thus, there is a smaller range for $K$ in the right hand column, and a wide range for $B$ in the left hand column. This could have a very critical impact on parameter estimation, since slanted confidence ellipsoids could be indicative of parameter dependence. The closer the ellipse is to a 90 degree angle, the more indicative of independence. Thus, in Figure 3 asymptotic ellipsoids suggest that the A-B parametrization produces correlated parameters.

6.2 Exact vs. asymptotic confidence ellipsoids

That there is little difference between the exact and asymptotic ellipsoids for the independent parametrizations of (7) is depicted in Figure 4. Exact confidence ellipsoids are not portrayed for the A-B parametrization presented in (8) because the cost functional in equation (21) created singular matrices, implying that the A-B parametrization was too correlated to effectively evaluate.

As mentioned previously, as $n \to \infty$, the asymptotic and exact confidence ellipsoids should coincide. Using a value of $n = 100$, we would hope to see fairly similar results from the two confidence ellipsoids. For the logistic
Figure 4: Logistic Example: Plots of confidence ellipsoids with parameter set 1 on the top and parameter set 2 on the bottom. The exact ellipsoids are on the left and the asymptotic ellipsoids are on the right.

model, the exact and asymptotic confidence ellipsoids seem to converge very nicely, as they have same relative shapes. This is important because the exact confidence intervals are not necessarily ellipsoidal; the asymptotic ellipsoids are since the $(\vec{\theta} - \hat{\theta})$ term is squared, which guarantees a parabolic shape. The exact confidence ellipsoids are smaller than the asymptotic confidence ellipsoids from both the r and K perspective. Notice the exact confidence interval on the top left of Figure 4 only extends from 8.15-7.75 on the y-axis, while its asymptotic counterpart extends from 8.5 to 7.25 (approximately). This trend is also seen on the bottom two graphs on both axis to a lesser extent. This would make sense given how the asymptotic method involves a linearization of parameters, which results in a loss of information and thereby a bigger margin in which the estimated parameters can occur with r level of confidence.

7 Parameter Distribution Results

7.1 Logistic Model

The logistic model parameterizations were quite obviously distributed in Figures 5 and 6. These graphs depict 1000 inverse problems ran on each parameter set for each noise level in the logistic model. The correlation is strongly evident in the A vs. B plots on the left hand side for all noise levels and both parameter sets, while the right sides are much more scattered and hence determined to be independent. This is true for both parameter sets.

7.2 Spring Model

The graphs in Figures 7 and 8 depict 1000 inverse problems ran on each parameter set for each noise level with the spring model. The correlation between parameters here is essentially indistinguishable as compared to the preceding logistical model parameter distributions. This may be attributed to the more implicit way that the spring model was reparameterized in the C-ω. There is some barely visible correlation between the C – K plots
Figure 5: Logistic Example: Plots of 1000 sets of A-B (left) and r-K (right) for parameter set 1. Going from top to bottom, the noise levels are 0.01, 0.05, and 0.20.
Figure 6: Logistic Example: Plots of 1000 sets of A-B (left) and r-K (right) for parameter set 2. Going from top to bottom, the noise levels are 0.01, 0.05, and 0.20.
for parameter set 1, but this is definitely a stretch in parameter set 2. Therefore, it is possible to conclude that both of these parameterizations are independent.
Figure 7: Spring Example: Plots of 1000 sets of C-K (left) and C-\(\omega\) (right) for parameter set 1. Going from top to bottom, the noise levels are 0.01, 0.05, and 0.20.
Figure 8: Spring Example: Plots of 1000 sets of C-K (left) and C-ω (right) for parameter set 2. Going from top to bottom, the noise levels are 0.01, 0.05, and 0.20.
8 Conclusions

In this project, we sought to answer whether or not we could distinguish between independent and dependent parametrizations in mathematical models. Although this study can help in determining independence of parametrizations, it could also aid in the direction for a study to determine the best possible parametrization for a given mathematical model. In our study we algebraically manipulated the underlying differential equations in order to change parametrizations. Another option is offered in [4], where a curvature array is defined and then used to define nonlinear equations to reduce correlation between parameters. We have taken two well known mathematical models and analyzed the effects on parameter estimation through several different simulated data sets. In looking at the covariance matrices and comparing each parametrization, no distinguishable factors can be found in these covariance matrices. However it is possible to demonstrate that there is evidence of parameter dependency that can be seen from asymptotic theory ellipsoids. This is evident in the logistic model case, where the parameter distribution results clearly show parameter dependence for the $A - B$ case, but not in the $r-K$ parametrizations.

This project suggests a possible way of by-passing the time-consuming Bayesian and Monte Carlo methods of uncertainty quantification. The results of the covariance matrices were too similar between different parameterizations to be distinguishable or conclusive. But as evidenced by the A-B parametrization of the logistic model, there was dependence exhibited in both the confidence ellipsoids and the parameter distributions while no distinguishing factors were found in the covariance matrices. Therefore, while other methods of uncertainty quantification may be able to detect which parameterizations are “better” when developing a mathematical model, the method of asymptotic covariances matrices produces dubious results.

We also compared asymptotic and exact confidence ellipsoids and determined that for the logistic model, the asymptotic ellipsoids seemed to imitate the exact ellipsoids very closely, especially for a fairly large value of $n = 100$. It may be more appropriate to use the exact method when creating confidence ellipsoids, as these ellipsoids should be more accurate than the asymptotic confidence ellipsoids due to their formulation, and they do not require the large number of experimental data points that an asymptotic confidence ellipsoid sometimes requires.

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