Reduced Cost Mission Design Using Surrogate Models

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Abstract

This paper uses surrogate models to reduce the computational cost associated with spacecraft mission design in three-body dynamical systems. Sampling-based least squares regression is used to project the system response onto a set of orthogonal bases, providing a representation of the ΔV required for rendezvous as a reduced-order surrogate model. Models are presented for mid-field rendezvous of spacecraft in orbits in the Earth-Moon circular restricted three-body problem, including a halo orbit about the Earth-Moon L_2 libration point (EML-2) and a distant retrograde orbit (DRO) about the Moon. In each case, the initial position of the spacecraft, the time of flight, and the separation between the chaser and the target vehicles are all considered as design inputs. The results show that sample sizes on the order of 10^2 are sufficient to produce accurate surrogates, with RMS errors reaching 0.2 m/s for the halo orbit and falling below 0.01 m/s for the DRO. A single function call to the resulting surrogate is up to two orders of magnitude faster than computing the same solution using full fidelity propagators. The expansion coefficients solved for in the surrogates are then used to conduct a global sensitivity analysis of the ΔV on each of the input parameters, which identifies the separation between the spacecraft as the primary contributor to the ΔV cost. Finally, the models are demonstrated to be useful for cheap evaluation of the cost function in constrained optimization problems seeking to minimize the ΔV required for rendezvous.

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These surrogate models show significant advantages for mission design in three-body systems, in terms of both computational cost and capabilities, over traditional Monte Carlo methods.

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1. Introduction

In the modeling of complex systems, a trade-off typically exists between computational expense and model fidelity. This holds true for the design of high thrust rendezvous missions in complex astrodynamical systems. For these systems, no explicit solution exists for the acceleration acting on a spacecraft, and trajectory design and optimization methods traditionally rely on iterative integration of a system of ordinary differential equations (ODEs). Much recent effort has been focused on developing improved techniques for low thrust trajectory optimization in such systems (see [Peng et al. \(2011, 2013\)](#); [Pontani et al. \(2012\)](#); [Pontani and Conway \(2012\)](#), among others). However, some missions - particularly crewed missions - require the use of high thrust spacecraft; the current concept of operations for the Asteroid Redirect Mission (ARM), for example, calls for the rendezvous of the crewed Orion spacecraft with the Asteroid Redirect Vehicle (ARV) using impulsive maneuvers ([Hinkel et al., 2014](#)). Some recent work has been done in the area of high thrust design and optimization ([Pontani et al., 2012](#)), including the use of surrogate models for interplanetary transfer trajectories ([Gano et al., 2006](#)). This paper considers a more robust approach to surrogate model development in order to provide an accurate and efficient method for the characterization and optimization of the design space for high thrust spacecraft trajectories.

Surrogate models address the trade-off between accuracy and computational expense by representing the system by a reduced-order model, which minimizes the need for repeated evaluation of an ODE solver and other computationally expensive techniques during analysis ([Simpson et al., 2001a](#); [Queipo et al., 2005](#); [Jin et al., 2001](#)). Surrogate models have been proven to be an effective means of representing and estimating complex systems involving both large numbers of design variables and inherent uncertainty. This paper applies surrogate models to the design of impulsive spacecraft rendezvous maneuvers, taking advantage of the models' ability to represent

complex trade spaces for rapid analysis and optimization. The paper explores the ability of surrogate models to aid in the mission design process in the context of spacecraft rendezvous in the Earth-Moon circular restricted three-body system, including spacecraft in halo orbits about the Earth-Moon L_2 libration point (EML-2) and in distant retrograde orbits (DRO) about the Moon. The complex nature of the three-body system precludes the use of analytical approximations, necessitating numerical simulations and creating an opportunity for reduced computational cost using the surrogate models. The use of these models as efficient design tools can enable significant time savings when performing, for example, trajectory design over long propagation times, trajectory optimization using massive grid searches, or trade space exploration for exercises in rapid mission design. Further, while optimization techniques such as the interior-point algorithm can determine an optimal solution for approximately the same computational cost as that associated with building and validating the surrogate model, the surrogate provides more comprehensive information about the system as a whole rather than an isolated optimal solution, including the number and location of local minima, location of the global minimum, and the absolute and relative effects of changes in each of the design parameters on the resulting ΔV . The development of rapid trajectory design and optimization tools such as these were identified by [Quadrelli et al. \(2013\)](#), in particular, as a priority for enabling future planetary science missions.

Many types of surrogate models have been developed for design, optimization, and analysis, including, for example, polynomial regression/interpolation ([Draper and Smith, 1998](#); [Boyd, 2001](#)), Kriging ([Matheron, 1963](#); [Simpson et al., 2001b](#); [Queipo et al., 2005](#)), and radial basis functions (see [Buhmann \(2000\)](#) for a survey of the the radial basis methods). In each case, the surrogate model seeks to use a relatively small number of sample points to generate a global function capable of approximating the system response for a reduced computational cost compared to traditional Monte Carlo methods. In addition to reducing the computational cost, surrogate models provide the ability to perform sensitivity analysis of the system on the input parameters under consideration.

Regardless of the the specific model chosen, the model development process includes three steps common to all surrogate models: design of experiments (DOE), estimation of the surrogate, and model validation ([Queipo et al., 2005](#); [Koziel et al., 2011](#)). The DOE involves the selection of the sample points used to generate realizations of the solution of interest, also known

as the training data. In model estimation, the true system response is solved for at each of the sample points selected in the DOE, and these solutions are then used to estimate the parameters that describe the surrogate. Finally, the resulting model is validated by assessing its predictive capabilities and performing error analysis. Although it is conceptually convenient to describe the model development as a sequential process, it should be noted that the process is frequently non-linear and iterative in practice.

This paper takes a comprehensive approach to the model development process for modeling the impulsive ΔV required for spacecraft rendezvous in the circular restricted three-body problem (CRTBP) as a function of deterministic design inputs. In the DOE, a novel sampling method developed in [Hampton and Doostan \(2014, 2015\)](#) is introduced, which is shown to lead to more rapid convergence of the model solution and is therefore demonstrated to be superior to classical sampling approaches. In model estimation, least squares regression is selected as the model of choice due to the adaptability of its basis functions to best suit the system under consideration. These functions can be chosen according to the boundary conditions associated with deterministic design inputs, as is done here, or alternatively, if the surrogate is mapping uncertainties in stochastic input parameters through a dynamical system, the bases can be selected according to the probability distribution of those stochastic inputs ([Wiener, 1938](#); [Ghanem and Spanos, 1991](#)). This method, known as polynomial chaos (PC) expansions, is very useful for uncertainty quantification and propagation ([Xiu, 2010](#); [Le Maître and Knio, 2010](#)). It has the potential to be combined with non-stochastic regression models for the purpose of optimization under uncertainty (OUU) ([Eldred, 2009, 2011](#)). Thus, another benefit of using regression modeling for this work is to serve as the foundation for future work in developing an accurate and cost-effective method for OUU as applied to spacecraft maneuver design. Finally, in model validation, this paper considers two separate validation data sets, one useful for providing a comprehensive analysis of the modeling errors and the other more conducive to rapid, autonomous model development. This comprehensive approach, which considers the complexities in the sampling scheme required to achieve desired accuracies, the flexibility and black box functionality provided by the regression model, and the autonomy provided by the k -fold validation scheme, results in a single tool that provides a unique approach to high thrust trajectory design and optimization.

Section 2 of the paper provides a review of the dynamics of the CRTBP and defines the orbits to be considered for the rendezvous problem. Sec-

tion 3 includes the relevant background needed for generating a surrogate using least squares regression, including the design of experiments, model estimation, and model validation, in addition to introducing a technique for global sensitivity analysis enabled by the surrogate. The results of the models built for rendezvous in both a halo orbit and a DRO are presented in Section 4, where these results are also applied to a constrained optimization of the rendezvous maneuver.

2. Problem Setup

This paper is concerned with spacecraft in the Earth-Moon three-body system and particularly considers the dynamics defined by the CRTBP. Thus, the system dynamics of interest for the model are, in dimensionless form,

$$\begin{aligned}\ddot{x} - 2\dot{y} - x &= -\frac{(1-\mu)(x-\mu)}{r_1^3} - \frac{\mu(x+1-\mu)}{r_2^3} \\ \ddot{y} + 2\dot{x} - y &= -\frac{(1-\mu)y}{r_1^3} - \frac{\mu y}{r_2^3} \\ \ddot{z} &= -\frac{(1-\mu)z}{r_1^3} - \frac{\mu z}{r_2^3},\end{aligned}\tag{1}$$

where

$$r_1 = \sqrt{(x+\mu)^2 + y^2 + z^2}, \quad r_2 = \sqrt{(x+\mu-1)^2 + y^2 + z^2}$$

and μ is the mass ratio of the Earth-Moon system,

$$\mu = \frac{m_M}{m_E + m_M}.$$

A surrogate model is first built for spacecraft orbiting in a 10,000 km z -amplitude halo orbit about the EML-2 libration point, as illustrated in Fig. 1. Specifically, the surrogate is used to model the mid-field rendezvous phase, in which a two-burn sequence carries the chaser vehicle from orbit insertion to the start of its proximity operations with the target (Hinkel et al., 2014). The design inputs include the initial position of the chaser vehicle, as measured by the τ -value (see Fig. 1(a)); the separation between the chaser and target vehicles $\Delta\tau$; and the time of flight t . Table 1 presents the range of values considered for these design parameters. The quantity of interest to be modeled is the ΔV required for rendezvous, including the magnitude

Table 1: Rendezvous design space

	Range		
	Halo	DRO ($d = 2$)	DRO ($d = 3$)
Initial position, τ ($^\circ$)	[0, 360]	0	[0, 360]
Time, t (days)	[0.25, 1]	[0.25, 1]	[0.25, 1]
Initial separation, $\Delta\tau$ ($^\circ$)	[0.1, 5]	[0.01, 0.25]	[0.01, 0.25]

of the total ΔV and the x -, y -, and z -components of the initial and final burns. Using the three design parameters, the deterministic solutions for the required ΔV are computed with a single-shooting differential corrector. Figure 2 shows the magnitude of the actual total required ΔV for rendezvous in the halo orbit.

Figure 1: 10,000 km z -amplitude halo orbit at EML-2

Once the surrogate framework is developed and refined for the halo orbit, it is next applied to mid-field rendezvous of spacecraft in a distant retrograde orbit (DRO) about the Moon in order to assess the model's capabilities as a black box development tool for three-body dynamics that requires minimal additional processing.

The orbit selected is a 70,000 km DRO, as shown in Fig. 3, of particular interest to NASA for its Asteroid Redirect Mission (ARM), in which the crewed Orion vehicle will rendezvous with an asteroid and the Asteroid Redirect Vehicle (ARV) already in orbit in the DRO. This case has previously

Figure 2: Total required ΔV for spacecraft rendezvous in a 10,000 km z-amplitude halo orbit about EML-2

been studied by [Hinkel et al. \(2014\)](#) using a Monte Carlo approach, and this paper aims to show that the use of a surrogate model can provide additional information and analysis capabilities over the Monte Carlo at a considerably reduced computational cost.

Figure 3: 70,000 km distant retrograde orbit about the Moon

In [Hinkel et al. \(2014\)](#), the ΔV cost of rendezvous is determined for space-

craft separated by $0.01 - 0.22^\circ$ for a single position τ , with a time of flight of 6, 12, or 24 hours. This paper first replicates the previous study, in which only $\Delta\tau$ and t are included as design dimensions, and then extends the study to include the initial position of the spacecraft as a third design dimension. The design parameters for each of these cases are also provided in Table 1. The true magnitude of the ΔV required for rendezvous in the DRO is given in Fig. 4, which illustrates that τ can have a non-negligible effect on ΔV that is not accounted for in Hinkel et al. (2014). While the shape of the function is very similar to that seen for the halo orbit, the case of the DRO results in lower required ΔV due to the smaller values of $\Delta\tau$ being used.

Figure 4: Total required ΔV for spacecraft rendezvous in a 70,000 km DRO

3. Overview of Surrogate Models

Accurate characterization and optimization of the design space for high thrust rendezvous requires a surrogate model of equivalent accuracy. A comprehensive approach to the development of a surrogate model is considered here in order to achieve desired levels of accuracy, as well as to maintain flexibility in the model framework such that it can be applied to a variety of mission scenarios. Surrogate models have a rich history in design and analysis for a variety of aerospace disciplines, including structural design (Barthelemy and Haftka, 1993), rocket engine component design (Farmer et al., 2000; Papila et al., 2002; Vaidyanathan et al., 2000), cavitating flows (Goel et al.,

2008), helicopter rotor blade vibrations (Glaz et al., 2009), and missile performance (Riddle et al., 2009). More recently, surrogate modeling has been applied to the field of astrodynamics, including interplanetary transfers and satellite constellation design (Gano et al., 2006), low thrust trajectory optimization (Peng et al., 2013), low thrust controls (Ghosh and Conway, 2013), and orbit uncertainty propagation (Jones and Doostan, 2013; Jones et al., 2013). This section provides the necessary background on surrogate models and the model development process for application to the problem of spacecraft rendezvous in the CRTBP.

3.1. Regression Modeling

Regression modeling expresses the functional dependence of a system response on the d -dimensional system inputs as a linear combination of a set of spectral basis functions ψ_i , resulting in the series expansion

$$u(\mathbf{s}) = \sum_{i=1}^{\infty} c_i \psi_i(\mathbf{s}), \quad (2)$$

where ψ_i are functions of the system inputs $\mathbf{s} = [s_1, s_2, \dots, s_d] \in \Gamma^d = [-1, 1]^d$, and c_i are the corresponding coefficients. This work considers basis functions ψ_i that are orthonormal, i.e.,

$$\int_{\Gamma^d} \psi_i(\mathbf{s}) \psi_j(\mathbf{s}) d\mathbf{s} = \delta_{ij},$$

where δ_{ij} is the Kronecker delta. In practice, under some regularity conditions, $u(\mathbf{s})$ can be approximated using (possibly small) P expansion terms, such that

$$u(\mathbf{s}) \approx u_P(\mathbf{s}) = \sum_{i=1}^P c_i \psi_i(\mathbf{s}), \quad (3)$$

for an appropriate ordering of the basis functions ψ_i . Thus, the modeling error $\varepsilon(\mathbf{s})$ associated with the surrogate is the truncation error given by

$$\varepsilon(\mathbf{s}) = \sum_{i=P+1}^{\infty} c_i \psi_i(\mathbf{s}). \quad (4)$$

The exact solution of the coefficients corresponding to the expansions in Eqs. (2) and (3) is the projection of the solution $u(\mathbf{s})$ onto the bases ψ_i ,

$$c_i = \langle u(\mathbf{s}) \psi_i(\mathbf{s}) \rangle = \int_{\Gamma^d} u(\mathbf{s}) \psi_i(\mathbf{s}) d\mathbf{s}, \quad (5)$$

where it is assumed that

$$\int_{\Gamma^d} u^2(\mathbf{s}) d\mathbf{s} < \infty.$$

When Eq. (5) is used to solve for the truncated model of Eq. (3), increasing the number of terms P results in mean-squares convergence of the estimate $u_P(\mathbf{s})$ to the true response $u(\mathbf{s})$, i.e.,

$$\langle (u(\mathbf{s}) - u_P(\mathbf{s}))^2 \rangle \rightarrow 0 \quad \text{as} \quad P \rightarrow \infty. \quad (6)$$

In multidimensional systems, the ψ_i of Eq. (3) are taken to be the tensor product of the univariate basis functions $\psi_{\alpha_k}(s_k)$ in each design dimension s_k , $k = 1, \dots, d$, such that

$$\psi_{\boldsymbol{\alpha}}(\mathbf{s}) = \psi_{\alpha_1}(s_1) \times \dots \times \psi_{\alpha_d}(s_d). \quad (7)$$

For polynomial bases, $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_d)$ denotes a multi-index defined for total order bases, for instance, by

$$\boldsymbol{\alpha} \in \Lambda_{p,d} = \{(\alpha_1, \dots, \alpha_d) \in \mathbb{N}_0^d : \|\boldsymbol{\alpha}\|_1 \leq p\},$$

for which α_k denotes the degree of the univariate polynomial function $\psi_{\alpha_k}(s_k)$, p is the total degree of the expansion, and $\mathbb{N}_0 = \{0, 1, 2, \dots\}$ is the set of natural numbers. The tensor-product basis construction in Eq. (7) allows for the basis functions ψ_{α_k} in each dimension s_k to be chosen independently (Soize and Ghanem, 2004). Eq. (3) may then be rewritten as

$$u_P(\mathbf{s}) = \sum_{\boldsymbol{\alpha} \in \Lambda_{p,d}} c_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\mathbf{s}). \quad (8)$$

The number of terms P in the resulting polynomial expansion is dependent on both p and the number of input dimensions d and is given by

$$P = |\Lambda_{p,d}| = \frac{(p+d)!}{p!d!}.$$

The enrichment of the approximation given by u_P in Eq. (8) is therefore achieved by increasing the total order of expansion p , which results in retaining a larger number of expansion terms P .

Many types of functions are available for use as the basis in spectral expansions. In regression modeling, ψ_i may be chosen to be orthogonal bases

dependent on the support of the design parameters (Boyd, 2001). Of particular interest here are problems with periodic boundary conditions, e.g. the initial τ of the chaser spacecraft in the rendezvous problem, and those with non-periodic boundary conditions defined over a finite interval, e.g. the $\Delta\tau$ and t dimensions in the same problem. Non-periodic systems with a finite domain may be represented using either Chebyshev or Legendre polynomials; Legendre polynomials have been selected for this work, such that the basis functions take the form

$$\psi_i(s) = L_i(s),$$

where $L_i(s)$ is the Legendre polynomial of degree i .

Periodic systems have been shown to be best modeled using a Fourier expansion, for which the non-constant basis functions are

$$\psi_i(s) \in \{\cos(i\pi s), \sin(i\pi s)\}.$$

Because the Fourier expansion contains both sine and cosine terms, however, the use of these bases in the expansion of Eq. (3) results in a number of terms equal to

$$P' = 2^{d_F} \cdot P - d_F,$$

where d_F is the number of design dimensions along which the solution is approximated with a Fourier expansion. Here, both the Fourier and Legendre bases are defined for $s \in [-1, 1]$.

3.2. Model Development Process

3.2.1. Design of Experiments

The primary concern of the design of experiments (DOE) is the sampling method used to select the training data, i.e., realizations of $\mathbf{s}$ and $u(\mathbf{s})$, with which to generate the surrogate model. Monte Carlo sampling provides a basic approach, in which the input data points are randomly selected over the design space Γ^d . Typically, the Monte Carlo points are generated from a sampling measure orthogonal to the basis functions used in the expansion. For both Legendre and Fourier bases, this corresponds to a uniform sampling of Γ^d .

Alternatively, a sampling measure associated with an asymptotic analysis of the orthogonal polynomials for large p is better suited for cases requiring high order polynomial approximations (Hampton and Doostan, 2015). In particular, this approach allocates more sample points near the boundaries

of the design space. The asymptotic measure associated with Legendre basis functions is the Chebyshev distribution (Rauhut and Ward, 2012). A Chebyshev sample is a realization of a random variable drawn from the distribution

$$f_c(s) = \frac{1}{\pi\sqrt{1-s^2}}, \quad (9)$$

for $s \in [-1, 1]$. If U is a random variable uniformly distributed on $[0, 1]$, $\cos(\pi U)$ follows the Chebyshev distribution, giving a method for sampling from this distribution. For both uniform and Chebyshev random sampling, each coordinate is drawn independently.

Modifications on traditional Monte Carlo sampling such as Latin hypercube sampling (LHS) and orthogonal arrays (OA) have been developed to reduce model bias and prevent clustering of data in the training set (Queipo et al., 2005), but these techniques do not allow for the reuse of data points when the size of the training set is adjusted to improve model accuracy. Another common approach to sampling uses a deterministic set of points to generate the model rather than random sampling; these techniques include, for example, pseudospectral collocation. However, this approach is subject to the curse of dimensionality, which states that the number of total function evaluations M grows exponentially with respect to the dimensionality d . Finally, other deterministic techniques such as A-, D-, and E-optimal seek to improve the stability of the linear system of Eq. (13) (discussed in the following section), from which the expansion coefficients are computed (Santner et al., 2003; Pukelsheim, 1993).

3.2.2. Estimation of the Model

The solution of the integral in Eq. (5) to generate the surrogate model is generally not straight-forward, and methods have been developed to determine a best estimate of the coefficients c_i using the system response at the training points selected in the DOE. Sampling-based methods achieve this estimation by relying only on the system inputs and outputs, thus treating the system solver as a black box. Two commonly-used sampling-based methods for generating a surrogate model are least squares regression and pseudospectral collocation. For the method of least squares, which is used here, $u(\mathbf{s})$ is evaluated at random sample points $\{\mathbf{s}^{(i)}\}$ and Eq. (3) is written in matrix form as

$$\mathbf{u} \approx \Psi \mathbf{c}, \quad (10)$$

where $\mathbf{u} = (u(\mathbf{s}^{(1)}), \dots, u(\mathbf{s}^{(M)}))^T$ is the vector of realizations of the system response at each of the M sample points $\mathbf{s}^{(i)}$, $\mathbf{c} = (c_1, \dots, c_P)^T$ is the vector of expansion coefficients, and Ψ is an $M \times P$ matrix containing evaluations of the basis functions for each term of the expansion at each sample. Using the notation $\{\psi_j\}$, $j = 1, \dots, P$, with a one-to-one correlation between $\{\psi_j\}$ and $\{\psi_\alpha\}$, the (i, j) -th element of Ψ is defined as

$$\Psi(i, j) = \psi_j(\mathbf{s}^{(i)}). \quad (11)$$

The least squares estimation, then, seeks to solve for $\mathbf{c}$ such that the sum of the squares of differences between the model prediction $u_P(\mathbf{s})$ and the system response $u(\mathbf{s})$ is minimized at the M sample points, or

$$\hat{\mathbf{c}} = \arg \min_{\mathbf{c}} \|\mathbf{u} - \Psi \mathbf{c}\|_2^2. \quad (12)$$

This corresponds to the solution of the normal equation

$$(\Psi^T \Psi) \hat{\mathbf{c}} = \Psi^T \mathbf{u}. \quad (13)$$

For samples taken according to the Chebyshev distribution for high order approximations, an adjustment must be made to the computation in Eq. (13) to compensate for the lost of orthogonality between the polynomials and the sampling measure when determining the least squares solution, as explained in detail in [Hampton and Doostan \(2015\)](#). Specifically, if $s_k^{(i)}$ denotes the realization of a sample in the k th coordinate of a sample $\mathbf{s}$, then let

$$w(\mathbf{s}^{(i)}) = \prod_{k=1}^d (1 - (s_k^{(i)})^2)^{1/4}. \quad (14)$$

For each realized $\mathbf{s}^{(i)}$, there is a corresponding row of Ψ and a corresponding entry of $\mathbf{u}$. For the computation in Eq. (13), both of these are multiplied by $w(\mathbf{s}^{(i)})$. That is, Eq. (13) is instead computed by

$$(\Psi^T \mathbf{W}^2 \Psi) \hat{\mathbf{c}} = \Psi^T \mathbf{W} \mathbf{u}, \quad (15)$$

where $\mathbf{W}$ is a positive diagonal matrix with entries $w(\mathbf{s}^{(i)})$.

For a discussion on the analysis of least squares regression and the required number of samples M for successful solution recovery, the interested reader may refer to [Cohen et al. \(2013\)](#) and [Hampton and Doostan \(2014\)](#).

Related to least squares regression, recent techniques based on compressive sampling exploit the sparsity in $\mathbf{c}$ to reduce M , and hence the computation cost, required for a successful solution recovery (Doostan and Owhadi, 2011; Hampton and Doostan, 2014).

Finally, while the construction of the surrogates was described here in the context of a scalar quantity of interest (QOI), the technique can also be applied to vector-valued QOIs with no required increase in M . For N QOIs, the vector $\mathbf{u}$ in Eq. (10) becomes an $M \times N$ matrix, and, similarly, the estimated matrix $\mathbf{c}$ is of dimension $P \times N$. Additional information on surrogate solutions for vector-valued QOIs can be found in Jones and Doostan (2013).

3.2.3. Validation

The third step in the model development process involves assessing the ability of the model to accurately predict the true system response. Inherent in this step is the selection of the validation data set, which is ideally independent of the data used in the construction of the surrogate model. Model validation is useful in gaining a more complete understanding of any modeling errors and, if multiple surrogates are being considered, in the selection of the surrogate best suited for the system.

To enable more robust analysis during the initial evaluation of the suitability of least squares regression in modeling impulsive maneuvers in the CRTBP, the models developed here are first compared to a very large validation set consisting of a grid of data points uniformly distributed along each input dimension, for a total number of points on the order of 10^5 for the case of the halo orbit and 10^4 for the DRO. The grid size in each dimension, as well as total number of resulting validation points, are provided in Table 2. Using these points, the models are evaluated based on the RMS validation errors, calculated as

$$\varepsilon_2 = \sqrt{\frac{1}{M_v} \sum_{i=1}^{M_v} (u_P(\mathbf{s}^{(i)}) - u(\mathbf{s}^{(i)}))^2}, \quad (16)$$

where M_v is the number of validation points, $u_P(\mathbf{s}^{(i)})$ is the model estimate at these points, and $u(\mathbf{s}^{(i)})$ is the true value at each point.

This approach to model validation, though, is clearly not practical for general applications and rapid model development. Other methods have

Table 2: Validation data sets

	Step Size			Total Number of Points
	Initial Position, τ ($^{\circ}$)	Time, t (days)	Initial Separation, $\Delta\tau$ ($^{\circ}$)	
Halo Orbit	2	0.05	0.1	144800
DRO	2	0.05	0.01	72400

been designed for model validation which impose less computational cost while still providing a thorough and unbiased assessment of the model errors, e.g. k -fold cross-validation and bootstrapping, among others (Geisser, 1975; Queipo et al., 2005). In particular, k -fold cross-validation, applied in this study, has the advantage of allowing all available sample data to be used for both constructing and validating the surrogate model. The process for k -fold validation is as follows:

1. Divide the training data set of size M into k subsets of approximately equal size.
2. Construct k surrogates, each omitting one subset of data to be used as the validation set.
3. Compute the model error for each estimated surrogate against its corresponding validation set.
4. Average the model error from each of the k surrogates to obtain the generalization error estimate.
5. If the generalization error estimate falls within accuracy requirements, generate a final surrogate using all M data points.

Further, the k -fold cross-validation technique can be combined with the sampling and estimation methods outlined above to enable autonomous model development. This algorithm begins with a first order expansion, uses Monte Carlo samples from the appropriate distributions to generate a model using least-squares regression, and calculates the k -fold RMS error. If the k -fold error does not meet accuracy requirements, the number of samples is increased incrementally, and a new model is generated and assessed for each new sample size. If the sample size reaches the threshold

$$M \geq \gamma \cdot P_{current}, \quad (17)$$

where

$$P_{current} = \frac{(p_{current} + d)!}{p_{current}!d!}$$

and γ is a design parameter, the expansion order of the model is also increased, so that

$$p_{new} = p_{current} + 1. \quad (18)$$

The process is then repeated until the resulting modeling error meets the specified accuracy requirements. This adaptive method allows for the generation of models with no *a priori* knowledge on either the required order of expansion or the sample size necessary for convergence.

3.3. Analysis of Variance

Once built, surrogates can, among other uses, be utilized to conduct analysis of variance (ANOVA) for the solution of interest. ANOVA techniques are methods which provide a measure of the global sensitivity of the QOI of a system to variations in each of the system inputs. One commonly used measure, the Sobol' sensitivity indices (Sobol', 1993), was developed in the context of stochastic systems and represents sensitivities as a ratio of the variance in the QOI due to stochastic dimension i to the total variance,

$$S_i = \frac{D_i}{D}. \quad (19)$$

Although these indices can be calculated via Monte Carlo simulation, a method introduced in Sudret (2008) makes use of polynomial chaos surrogates to enable an analytic computation of the indices using the expansion coefficients.

While design surrogates are not stochastic and therefore the approach in Sudret (2008) is not directly transferable to the models developed here, a related set of indices is proposed in which the indices provide a relative measure of the dependence of the system response on input i and are defined as

$$S_i = \frac{C_i}{C}, \quad (20)$$

where

$$C_i = \sum_{\alpha_i \in \Lambda_{p,d}} c_{\alpha_i}^2, \quad (21)$$

α_i is the multi-index in $\Lambda_{p,d}$ for which the i th entry is non-zero, and

$$C = \sum_{i=1}^d C_i. \quad (22)$$

These sensitivity indices provide two specific advantages for sensitivity analysis. First, the indices can be calculated analytically with the expansion coefficients rather than empirically using a Monte Carlo method. Second, while many approaches to sensitivity analysis, such as function derivatives, provide information on local sensitivities, the indices of Eq. (20) can instead be used for global analysis. In effect, $\{S_i\}_{i=1}^d$ represent the overall contribution of each dimension to the system as a whole. In the context of spacecraft rendezvous, such an analysis provides useful information regarding which design inputs contribute most to the required ΔV and therefore which are the most important considerations for minimizing fuel costs during mission design.

4. Model Results

In this section, numerical simulations are used to build a surrogate of the ΔV (including the x -, y -, and z -components of the initial and final burns, as well as the total ΔV) required for spacecraft rendezvous and to assess the model's ability to accurately represent rendezvous in the three-body system. The full validation sets are used to evaluate the model performance in both the halo orbit and the DRO, including the magnitude and behavior of modeling errors. k -fold validation is then used to test the application of an algorithm for adaptive, autonomous model development.

4.1. Uniform Sampling in a Halo Orbit

A surrogate is first built for the case of rendezvous in the 10,000 km halo orbit using Fourier bases in the periodic τ dimension and Legendre bases in the t and $\Delta\tau$ dimensions, which are both non-periodic and defined over a finite interval. Figure 5 shows the RMS validation error of the model for the total ΔV as a function of the expansion order and sample size, averaged over 100 independent data sets for each sample size. It is readily evident that, as the order of the expansion increases, the approximation error decreases, until it reaches an error floor with a 9th order expansion. The larger errors associated with the lower order expansions correspond to the truncation error

defined in Eq. (4). As the order of the expansion approaches infinity, or, in the case of lower order dynamic systems, as the expansion order approaches the true system order, the truncation error should approach zero.

Figure 5: RMS validation errors averaged over 100 independent data sets using Monte Carlo sampling from a uniform distribution for rendezvous in a halo orbit

The error floor, which levels off at about 0.18 m/s for large sample sizes, has three potential sources. First, because the truth data used to initialize the model is generated by numerical simulations, any round-off errors in the simulation will translate into errors in the surrogate. The accuracy levels of the single-shooter being used, though, would suggest that numerical errors contribute very little, if any, to the error floor seen here. The more likely source of the error stems from the rapid decay in the true ΔV along the time dimension t as evidenced in Fig. 2. Generalized spectral expansions based on global smooth polynomials such as Legendre polynomials are recognized in [Le Maître et al. \(2004\)](#) to face difficulties in accurately modeling a steep dependence of the QOI on an input parameter. Finally, because of this behavior in the time dimension, there simply may not exist a more accurate, low order representation of the system; rather, a very high order expansion may be required to completely capture the system response.

Despite this floor, the modeling errors drop below 0.25 m/s using on the order of only 10^2 training points. For example, a 9th order expansion generated with 700 samples produces a validation error of 0.226 m/s. This expansion order results in $P = 385$ terms, and the corresponding coefficients can be found in Fig. 6. The drop in the coefficients of almost four orders

Figure 6: Coefficients for a 9th order polynomial expansion, normalized to the first term coefficient, as constructed from 700 uniform Monte Carlo samples for rendezvous in a halo orbit

Figure 7: Model results of a 9th order polynomial expansion using 700 Monte Carlo samples from a uniform distribution for rendezvous in a halo orbit at $\Delta\tau = 3^\circ$

Figure 8: RMS validation errors averaged over 100 independent data sets using Monte Carlo sampling from a uniform distribution in the τ dimension and from a Chebyshev distribution in the t and $\Delta\tau$ dimensions for rendezvous in a halo orbit

4.2. Chebyshev Sampling in a Halo Orbit

A comparison of Figs. 5 and 8 indicates that the use of Chebyshev, rather than uniform, random sampling in the t and $\Delta\tau$ dimensions leads to more rapid convergence of the model errors, particularly for higher order expansions. Specifically, in the 9th order expansion considered previously, the substitution of Chebyshev sampling results in a slightly smaller RMS validation error (0.207 m/s) using only 500 samples, almost 30% fewer than when uniform sampling was used in all three dimensions. Even more significant than the convergence rate of the validation errors is the variance of the error over the 100 data sets. Figure 9 shows that the variance in the RMS is reduced by almost an order of magnitude when Chebyshev sampling is used.

Chebyshev sampling is therefore taken to be the superior sampling method associated with Legendre bases for the rendezvous application considered here. The coefficients for a 9th order expansion from 500 training samples, shown in Fig. 10, are very similar to those in Fig. 6 and reach the same level of convergence. Figure 11(b) shows the model errors at $\Delta\tau = 3^\circ$, which are indeed smaller than those associated with uniform sampling in Fig. 7(b) above.

In computing the required ΔV for rendezvous, a single function evaluation using the surrogate model is up to two orders of magnitude faster than when using the full fidelity propagators. Further, the matrix form of Eq. (15) allows

Figure 9: Variance of the RMS validation errors for 100 independent data sets for rendezvous in a halo orbit

Figure 10: Coefficients for a 9th order polynomial expansion, normalized to the first term coefficient, as constructed from 500 Monte Carlo samples from a uniform distribution in the τ dimension and from a Chebyshev distribution in the t and $\Delta\tau$ dimensions for rendezvous in a halo orbit

for simultaneous evaluation of the surrogate for multiple design inputs, such that the marginal cost of computing the solution at multiple design points is negligible. Thus, significant cost savings over traditional propagators are accumulated when modeling the variation of the ΔV over the design space.

One limitation still present in the model is its difficulty in accurately predicting system behavior at the boundaries of the design space. In Fig. 11(b),

Figure 11: Model results of a 9th order polynomial expansion using 500 Monte Carlo samples from a uniform distribution in the τ dimension and from a Chebyshev distribution in the t and $\Delta\tau$ dimensions for rendezvous in a halo orbit at $\Delta\tau = 3^\circ$

Figure 12: Model results of a 9th order polynomial expansion using 500 Monte Carlo samples from a uniform distribution in the τ dimension and from a Chebyshev distribution in the t and $\Delta\tau$ dimensions for rendezvous in a halo orbit at $\Delta\tau = 0.1^\circ$

for example, the largest errors are concentrated near $t = 0.25$ days. Similarly, comparing Fig. 11 to Fig. 12, the model is clearly better able to capture the system response at a separation of $\Delta\tau = 3^\circ$ than at the boundary value of $\Delta\tau = 0.1^\circ$. This behavior indicates that a higher order solution is required to fully capture the system response at these boundaries, as evidenced by the periodic nature of the errors, with an associated increase in computational cost. Although the magnitude of the errors at $\Delta\tau = 0.1^\circ$ is generally small (see Fig. 12(b)), they may affect performance in applications such as

optimization and are therefore worth noting. Finally, Fig. 13 shows the component-wise errors for the initial and final burns. The errors, which are smaller than those corresponding to the magnitude of the total ΔV , are predominantly concentrated in the y -direction and are largest for short transfer times.

Figure 13: Component-wise model errors of a 9th order polynomial expansion using 500 Monte Carlo samples from a uniform distribution in the τ dimension and from a Chebyshev distribution in the t and $\Delta\tau$ dimensions for rendezvous in a halo orbit at $\Delta\tau = 3^\circ$

As noted, however, the full data set used for the validation of the previous two models is not generally available when developing the surrogate. Therefore, with the alternate sampling method in place for the DOE, a new model is developed for rendezvous in the halo orbit using the autonomous model generator and k -fold validation scheme outlined above, with $k = 10$ candidate surrogates. Figure 14 shows the convergence of the k -fold RMS error as a function of sample size. Increases in the expansion order are clearly evident in the step decreases in the RMS error, while increases in the sample size within a given order generally do not improve the model accuracy. Additionally, the k -fold errors appear to reach smaller values than the errors seen when using the full validation set, likely due to the spatial concentration of the larger modeling errors which are thus less likely to be represented in the smaller k -fold set compared to the full set. The k -fold RMS accuracy

requirement, then, is set to 0.05 m/s, and the model generator converges on a solution using a 9th order expansion with $M = 620$ training samples; when compared to the full validation set, the model results in an RMS error of 0.1957 m/s. Figure 15 contains the model and its errors at $\Delta\tau = 3^\circ$, which are very similar to the results obtained from the fixed order model.

Figure 14: k -fold RMS errors with $k = 10$, using Monte Carlo sampling from a uniform distribution in the τ dimension and from a Chebyshev distribution in the t and $\Delta\tau$ dimensions for rendezvous in a halo orbit

Figure 15: Model results after k -fold convergence with $k = 10$, using Monte Carlo samples from a uniform distribution in the τ dimension and from a Chebyshev distribution in the t and $\Delta\tau$ dimensions for rendezvous in a halo orbit at $\Delta\tau = 3^\circ$

4.3. Chebyshev Sampling in a DRO

In order to show the black box functionality of the model framework developed above for general applications in the three-body system, it is next applied to the 70,000 km DRO considered in [Hinkel et al. \(2014\)](#). The results presented here are obtained by simply changing the input conditions for the target and chaser vehicles, i.e., no additional development cost is required for modifications to the modeling tool. The only additional computational cost involved is that associated with the generation of new samples to build a model specific to this application.

In the NASA study, a Monte Carlo simulation is used to conduct an analysis of the total ΔV cost of mid-field rendezvous for the Asteroid Redirect Mission (ARM), in which the Orion vehicle uses a two-burn sequence to rendezvous with the Asteroid Redirect Vehicle (ARV). The study considers spacecraft separated by approximately $0.01 - 0.22^\circ$ from a single initial position, with discrete rendezvous times of 6, 12, and 24 hours. Solutions are presented for approximately 100 isolated points for which the Orion vehicle is initially trailing the ARV and about the same number of points for which the Orion is ahead of the target.

Figure 16 shows that using the models developed here for the case considering only the t and $\Delta\tau$ design dimensions with Legendre bases in each, very accurate surrogates can be built with fewer training samples than the ~ 100 points examined in [Hinkel et al. \(2014\)](#) for the case of the chaser trailing the target. In fact, an 8th order model achieves an RMS validation accuracy of $< 10^{-2}$ using only 60 samples, resulting in a full dynamical model for only about half the cost of the limited Monte Carlo analysis. In particular, the model reveals variations in the τ dimension which are missed in the previous study.

Figure 17 presents the validation errors with τ included as a third design dimension for the DRO, using Fourier bases in that dimension. While the model is still able to achieve accuracies comparable to the two-dimensional case, it requires on the order of 10^2 training samples to do so. The errors are much smaller than those seen in the case of the halo orbit, and the error floor that existed for the halo orbit is not present. Instead, the RMS error continually approaches 0 with increasing expansion order and sample size, a result of the smaller range of $\Delta\tau$ values under consideration.

From Fig. 17, a 9th order expansion generated from 500 training samples with an associated RMS error of 2.369×10^{-3} m/s is selected for further analysis. Figures 18 and 19 show the resulting model and its errors. Again,

Figure 16: RMS validation errors for rendezvous in a DRO with $d = 2$, using Monte Carlo sampling from a Chebyshev distribution in the t and $\Delta\tau$ dimensions

Figure 17: RMS validation errors for rendezvous in a DRO with $d = 3$, averaged over 100 independent data sets using Monte Carlo sampling from a uniform distribution in the τ dimension and from a Chebyshev distribution in the t and $\Delta\tau$ dimensions

the smaller range used in $\Delta\tau$ greatly improves the performance of the model, as seen in the shape of the predicted ΔV for the smallest separation angle.

Finally, with an accuracy requirement of 0.001 m/s, the k -fold-based generator once again converges on a 9th order expansion using 620 training samples. The model results for $\Delta\tau = 0.15^\circ$ can be found in Fig. 21. This last model is used to calculate the sensitivity indices of Eq. (20) for the design parameters in the DRO, and the results are shown in Table 3. From

Figure 18: Model results of a 9th order polynomial expansion using 500 Monte Carlo samples from a uniform distribution in the τ dimension and from a Chebyshev distribution in the t and $\Delta\tau$ dimensions for rendezvous in a DRO at $\Delta\tau = 0.01^\circ$

Figure 19: Model results of a 9th order polynomial expansion using 500 Monte Carlo samples from a uniform distribution in the τ dimension and from a Chebyshev distribution in the t and $\Delta\tau$ dimensions for rendezvous in a DRO at $\Delta\tau = 0.15^\circ$

these indices, the separation between the spacecraft has the largest impact on the ΔV cost of rendezvous, with the time of flight coming in second. Not surprisingly, the effect of the initial position within the orbit is, relatively, much smaller than that of the other two dimensions.

4.4. Maneuver Optimization

Although the primary purpose of the surrogate models developed in this section is to provide design data across the entire trade space, the represen-

Figure 20: k -fold RMS errors with $k = 10$, using Monte Carlo sampling from a uniform distribution in the τ dimension and from a Chebyshev distribution in the t and $\Delta\tau$ dimensions for rendezvous in a DRO

Figure 21: Model results after k -fold convergence with $k = 10$, using Monte Carlo samples from a uniform distribution in the τ dimension and from a Chebyshev distribution in the t and $\Delta\tau$ dimensions for rendezvous in a DRO at $\Delta\tau = 0.15^\circ$

tation of the required ΔV in the form of an explicit function of the design inputs also makes these surrogates ideally suited for cheap evaluation of the cost function in constrained optimization problems seeking to minimize the

Table 3: Sensitivity indices for rendezvous in a DRO

	τ	t	$\Delta\tau$
Sensitivity Index, S_i	0.0199	0.3872	0.5929

ΔV for spacecraft rendezvous. The optimization problem seeks to minimize the objective function $J(\mathbf{s})$, subject to equality constraints $\mathbf{F}(\mathbf{s})$:

$$\min_{\mathbf{s}} J(\mathbf{s}) = \sum_{\alpha \in \Lambda_{p,d}} c_{\alpha} \psi_{\alpha}(\mathbf{s}) \quad (23)$$

$$\begin{aligned} \text{s.t. } \mathbf{F}(\mathbf{s}) &= \mathbf{0} \\ \mathbf{s}_l &\leq \mathbf{s} \leq \mathbf{s}_u. \end{aligned}$$

The functional form of Eq. (23) enables easy generation of the Jacobian as

$$DJ = \frac{\partial u_p(\mathbf{s})}{\partial \mathbf{s}}. \quad (24)$$

The constrained minimization method used here is based on an interior point algorithm, which relies on determining a sequence of solutions to approximate minimization problems (see, for example, Byrd et al. (1999)). The interior point algorithm is implemented using Matlab’s *fmincon* optimizer.

Figure 22 shows the results of the optimizer applied to the problem of minimizing the total ΔV for rendezvous in the DRO over all three design inputs, τ , t , and $\Delta\tau$. Because *fmincon* is a local optimizer, two different results corresponding to the two local minima seen in Fig. 22 can be reached depending on the initial guess, and both are depicted in the figure. The identification of both local minima using a high fidelity differential corrector with the *fmincon* optimizer requires on the order of hundreds of function calls, although the actual number of calls varies significantly depending on the initial guess. This also assumes good *a priori* knowledge on both the number and general location of local minima. For cases with an unknown solution structure, the low computational cost associated with a polynomial cost function can facilitate the identification of the global minimum by conducting a survey of many initial guesses to identify all local minima.

Thus the surrogate model, which provides much more information across the design space than simply the isolated locations of the minimum ΔV ,

can be built and verified for approximately the same computational cost as the optimization of the ΔV using the full-fidelity solutions with *a priori* knowledge. Once the model is generated, it can be re-used for optimization under changing constraints throughout the mission design process, providing further cost savings. Finally, having identified the minimum total ΔV using surrogate-based optimization, the x -, y -, and z -components for each of the two burns can be extracted from the model, and these solutions can be used as initial guesses for high-fidelity optimization tools.

Figure 22: Optimized input parameters for minimum ΔV rendezvous in a DRO. Optimal solution occurred at $\Delta\tau = 0.01^\circ$

5. Conclusions

This paper applied the technique of surrogate modeling to mission design in the Earth-Moon three-body system. Specifically, the method of least squares regression was used to model the ΔV required for mid-field rendezvous of spacecraft in the Earth-Moon CRTBP, in both a halo orbit and a DRO. Additional savings in the number of samples required to generate the models were seen by using an asymptotic sampling measure, as opposed to the natural orthogonal sampling measures associated with the basis functions, resulting in the need for on the order of 10^2 training samples for the

case of three input design dimensions and fewer than 100 samples for the case of 2 design dimensions. Further, it was demonstrated that these surrogate models can be built with no *a priori* knowledge on either the expansion order or the sample size required for convergence. Once the surrogate was generated, the coefficients were used for an analytic global sensitivity analysis, and, finally, the model was shown to be ideally suited for use in evaluating the cost function for efficient maneuver optimization. The cases of rendezvous in a halo orbit and a DRO demonstrated the superiority of surrogate modeling over traditional Monte Carlo approaches in analysis capabilities and computational cost, with the cost of a single function evaluation using full fidelity propagators up to two orders of magnitude higher than when using the surrogate. Thus the surrogate model has been shown to be a useful tool for maneuver design and analysis in the CRTBP.

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