

# Learning and Optimization with Bayesian Hybrid Models

Elvis A. Eugene<sup>1†</sup>, Xian Gao<sup>1†</sup>, and Alexander W. Dowling<sup>1\*</sup>

**Abstract**—Bayesian hybrid models fuse physics-based insights with machine learning constructs to correct for systematic bias. In this paper, we compare Bayesian hybrid models against physics-based glass-box and Gaussian process black-box surrogate models. We consider ballistic firing as an illustrative case study for a Bayesian decision-making workflow. First, Bayesian calibration is performed to estimate model parameters. We then use the posterior distribution from Bayesian analysis to compute optimal firing conditions to hit a target via a single-stage stochastic program. The case study demonstrates the ability of Bayesian hybrid models to overcome systematic bias from missing physics with fewer data than the pure machine learning approach. Ultimately, we argue Bayesian hybrid models are an emerging paradigm for data-informed decision-making under parametric and epistemic uncertainty.

## I. INTRODUCTION

Both *model-based* and *data-driven* paradigms are regularly employed for control and decision-making [1], [2], [3], [4]. So-called glass-box (a.k.a., white-box) models [5], [6] are created from scientific theories, expert knowledge, and human intuition. They are regularly used to test scientific hypotheses and develop deeper fundamental understandings. When all dominant phenomena are included, glass-box models offer superior predictive power for extrapolation. Yet glass-box models are tedious to build and validate. With the availability of massive-scale data, black-box surrogate models [7], [8], [9], [10], [11], [12], [13], [14] are growing in popularity. Statistical machine learning paradigms are preferred over scientific theories for their ability to automate model (re)learning and extract undiscovered trends. At the intersection of these two paradigms are hybrid (a.k.a., grey-box) models which augment physics-based models with data-driven constructs to learn missing phenomena.

All mathematical models are burdened by uncertainty. *Aleatoric* or statistical uncertainty corresponds to random phenomena, such as variability between experiments or observation noise. In contrast, *epistemic* uncertainty corresponds to systematic bias or model inadequacy, such as omitting control variables in an experiment or missing physical phenomena in a model. Robust and stochastic model predictive control are well-established paradigms to accommodate parameter uncertainty [15]. Closely related, model-based design of experiments provides a principled approach to gather information to reduce parametric uncertainty, with recent work considering approximate models [16], [17]. From a data-driven perspective, Bayesian optimization [18] uses probabilistic surrogate models to manage exploration

(reducing model uncertainty) and exploitation (improving the objective). In this paper, we explore Kennedy-O’Hagan hybrid models as an alternative to pure glass-box and pure data-driven surrogate models.

The paper is organized as follows. In Section II, we define Bayesian hybrid models and review literature. In Section III, we demonstrate the advantages of hybrid models in an illustrative case study for Bayesian calibration and optimization with epistemic uncertainty. Finally, in Section IV, we summarize our conclusions and propose future work.

## II. BAYESIAN HYBRID MODELS

Statisticians Kennedy and O’Hagan [19] proposed a Bayesian framework to simultaneously quantify both aleatoric and epistemic uncertainty:

$$\underbrace{y_i}_{\text{observation}} = \underbrace{\eta(\mathbf{x}_i, \theta)}_{\text{glass-box model}} + \underbrace{\delta(\mathbf{x}_i; \phi)}_{\text{discrepancy model}} + \underbrace{\epsilon_i}_{\text{observation error}} \quad (1)$$

Here, observation  $y_i$  is modeled with three components: a glass-box model  $\eta(\cdot, \cdot)$  with physically meaningful global parameters  $\theta$  and inputs  $\mathbf{x}_i$  for experiment  $i$ ; a stochastic discrepancy function  $\delta(\cdot)$  to counteract systematic bias in the glass-box model; and observation error  $\epsilon_i$  such as uncorrelated white noise, i.e.,  $\epsilon_i \sim \mathcal{N}(0, \sigma^2 \mathbf{I})$ . Outputs of the Gaussian Process (GP) discrepancy function  $\delta(\cdot) \sim \mathcal{GP}(\mu(\cdot), k(\cdot, \cdot))$  follow a conditional normal distribution with the mean and covariance fully specified by  $\mu(\cdot)$ , the mean function, and  $k(\cdot, \cdot)$ , the kernel function, which include hyperparameters  $\phi$  [20], [21].

$$\underbrace{p(\omega|\mathcal{D})}_{\text{posterior}} = \frac{\overbrace{p(\mathcal{D}|\omega)}^{\text{likelihood}} \overbrace{p(\omega)}^{\text{prior}}}{\underbrace{\int p(\mathcal{D}|\omega)p(\omega)d\omega}_{\text{evidence}}} \quad (2)$$

For Bayesian model calibration, parameters  $\omega = [\theta, \phi, \sigma]$  are interpreted as random variables. One seeks to express their belief about the true value of  $\omega$  using a joint probability distribution. The standard workflow is to encode one’s current belief in a prior probability distribution, then observe data  $\mathcal{D}$ , and finally apply Bayes rule, Eq. (2), to obtain the posterior probability distribution  $p(\omega|\mathcal{D})$  [22]. For Eq. (1) and unobserved input conditions  $\mathbf{x}_i$ , the posterior distribution  $p(\theta, \phi, \sigma|\mathcal{D})$  can be propagated through  $\eta(\mathbf{x}_i, \theta)$ ,  $\delta(\mathbf{x}_i; \phi)$  and  $\epsilon_i$  to obtain the posterior predictive distribution  $p(y^*|\mathbf{y})$  for prediction  $y_i$ . Thus Kennedy and O’Hagan [19] provide a fully Bayesian framework to calibrate global model parameters  $\theta$ , quantify model inadequacy (i.e., systematic bias), and

<sup>1</sup>Department of Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN 46556 USA. <sup>†</sup> Contributed equally. \* Corresponding author: adowling@nd.edu

make probabilistic predictions. This is an extremely powerful and flexible approach that has been used in diverse fields such as computational fluid dynamics [23], electrochemical energy storage [24], and CO<sub>2</sub> capture [25], [26], [27], [28].

### III. ILLUSTRATIVE COMPUTATIONAL EXAMPLE

In this paper, we explore the performance of glass-box, data-driven, and hybrid models for decision-making. Specifically, we consider an illustrative problem of firing a ballistic to hit a desired target. We demonstrate Bayesian calibration and stochastic programming approaches for all three model classes using several training sets.

#### A. Mathematical Models

We start by describing the three mathematical models for the illustrative example. To avoid confusion with observations  $y_i$  in Eq. (1), we use  $x$  and  $z$  to represent horizontal and vertical positions, respectively. We consider a ballistic with mass  $m$  (kg) fired at the origin ( $x = 0$ ,  $z = 0$ ) at angle  $\psi$  ( $^\circ$ ) and initial velocity  $v_0$  (m/s).

1) *Glass-box, full physics model:* We start with four coupled differential equations and initial conditions to describe the ballistic trajectory. Here  $v_x$  and  $v_z$  correspond with the horizontal and vertical velocities (m/s), respectively.

$$m \frac{dv_z}{dt} = -mg - C_D v_z |v_z|, \quad (3)$$

$$m \frac{dv_x}{dt} = -C_D v_x^2, \quad (4)$$

$$\frac{dx}{dt} = v_x, \quad \frac{dz}{dt} = v_z, \quad (5)$$

$$\begin{aligned} v_x(0) &= v_0 \cos(\psi), & v_z(0) &= v_0 \sin(\psi), \\ x(0) &= 0, & z(0) &= 0. \end{aligned} \quad (6)$$

The full physics glass-box model, Eqs. (3) - (6), describes projectile motion while accounting for air-resistance effects. Model parameters include  $g$ , acceleration due to gravity (m/s<sup>2</sup>), and  $C_D$ , the coefficient of drag (kg/m). To account for the sign change in vertical velocity (i.e.,  $v_z$  decreases after being shot,  $v_z$  reaches zero at the projectile's peak height, and then increases during the projectile's downward motion), the first time domain (upward motion) and  $t \in [t_p, t_f]$  (downward motion). The absolute value in Eq. (3) ensures that the drag is always in the opposite direction of the vertical velocity vector. For the first time domain (upward motion), Eq. (3) becomes:

$$m \frac{dv_z}{dt} = -mg - C_D v_z^2, \quad (7)$$

$$v_z(0) = v_0 \sin(\psi), \quad v_z(t_p) = 0, \quad (8)$$

The above boundary value problem is analytically solved for the time  $t_p$  when the projectile reaches peak height and  $v_z(t_p) = 0$ . The analytic expression for  $t_p$  is given in Eq. (9).

$$t_p = \sqrt{\frac{m}{C_D g}} \arctan \left( v_z(0) \sqrt{\frac{C_D}{mg}} \right) \quad (9)$$

Next, we solve Eq. (10) to determine the peak height  $z(t_p)$ :

$$\begin{aligned} \frac{dz}{dt} &= v_z \\ v_z(0) &= v_0 \sin(\psi), \quad v_z(t_p) = 0 \end{aligned} \quad (10)$$

$$\begin{aligned} z(t_p) &= \\ \frac{m}{C_D} &\left( \ln \left( \left| \cos \left( \sqrt{\frac{C_D g}{m}} t - \arctan \left( \sqrt{\frac{C_D}{mg}} v_z(0) \right) \right) \right| \right) \right) \\ &- \ln \left( \left| \cos \left( \arctan \left( \sqrt{\frac{C_D}{mg}} v_z(0) \right) \right) \right| \right) \end{aligned} \quad (11)$$

The second time domain (downward motion) is described by Eqs. (12) - (13) and boundary conditions Eqs. (11) and (14).

$$m \frac{dv_z}{dt} = -mg + C_D v_z^2 \quad (12)$$

$$\frac{dz}{dt} = v_z \quad (13)$$

$$v_z(t_p) = 0, \quad v_z(t_f) = v_f, \quad z(t_f) = 0 \quad (14)$$

The analytic solution for this system is given by Eq. (15).

$$\begin{aligned} z(t_f) &= \sqrt{\frac{mg}{C_D}} \left( t_p - t_f + \left( \ln(2) \right. \right. \\ &\left. \left. - \sqrt{\frac{m}{C_D g}} \ln \left( \exp \left( 2 \sqrt{\frac{C_D g}{m}} (t_p - t_f) \right) + 1 \right) \right) \right) + z(t_p) \end{aligned} \quad (15)$$

To compute  $t_f$ , we set  $z(t_f) = 0$  and numerically solve Eq. (15). Finally, we use  $t_f$  in Eq. (16) to compute the total horizontal distance traveled. Our analysis assumes no change in elevation.

$$\hat{y}(t_f) = \frac{m}{C_D} \ln(C_D v_0 \cos \psi t_f + m) \quad (16)$$

$$y(t_f) = \hat{y}(t_f) + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma^2 \mathbf{I}) \quad (17)$$

In this paper, we use Eq. (17), which includes observation noise, in place of physical experiments.

We now describe three predictive surrogate models with inputs  $\mathbf{x}_i = [v_{0i}, \psi_i]$ , where  $v_{0i}$  is the initial velocity and  $\psi_i$  is the launching angle for experiment  $i$ . The input dimensionality is  $D = 2$ .

2) *Glass-box, simple physics surrogate model:* Often in engineering applications, the full physics model is not known, computationally intractable, or otherwise cumbersome to work with. Instead, a simplified surrogate model is often used. For the ballistics problem, we consider a parabolic trajectory that neglects air resistance:

$$y_i = \eta(\mathbf{x}_i, \theta) + \epsilon_i \quad (18)$$

$$\eta(\mathbf{x}_i, \theta) = \frac{2(v_{0i})^2}{g} \sin(\psi_i) \cos(\psi_i)$$

The impact location  $y$  (horizontal distance traveled) given by Eq. (18) does not depend on  $m$ , the projectile mass.

### 3) Black-box, Gaussian Process (GP) surrogate model:

Another approach is to construct a surrogate model completely from data, without incorporating (significant) knowledge or physical intuition. Here, we will consider  $y_i \sim \mathcal{GP}(\mu(\cdot), k(\cdot, \cdot))$ , i.e., a GP model with observation error:

$$y_i = \delta(\mathbf{x}_i; \phi) + \epsilon_i. \quad (19)$$

We use a Gaussian distribution with a zero mean and a covariance ( $\mathbf{K}$ ) constructed by the kernel function ( $k$ ) as a prior distribution for  $\delta$ :

$$p(\delta) = \mathcal{N}(\delta | \mathbf{0}, \mathbf{K}) \quad (20)$$

where  $\mathbf{K}_{mn} = k(\mathbf{x}_m, \mathbf{x}_n)$ . We use the radial-based function (RBF) with automatic relevance determination (ARD) [29]:

$$k(\mathbf{x}_m, \mathbf{x}_n) = \sigma_f^2 \exp\left[-\frac{1}{2} \sum_{i=1}^D \frac{(x_{mi} - x_{ni})^2}{l_i^2}\right] \quad (21)$$

where  $\sigma_f^2$  is the kernel variance and  $l_i$  is the lengthscale. Also a Gaussian likelihood is assumed for the  $N$  training data points:

$$p(\mathbf{y}|\delta) = \mathcal{N}(\mathbf{y}|\delta, \sigma^2 \mathbf{I}_N) \quad (22)$$

where  $\sigma^2$  is the variance of the observation noise. Using the properties of linear Gaussian models, one can derive the marginal likelihood function [20]:

$$p(\mathbf{y}) = \int p(\mathbf{y}|\delta)p(\delta)d\delta = \mathcal{N}(\mathbf{y}|\mathbf{0}, \mathbf{C}) \quad (23)$$

where  $\mathbf{C} = \mathbf{K} + \sigma^2 \mathbf{I}_N$ . Conditioning on the training data, we then derive the predictive distribution:

$$p(y^*|\mathbf{y}) = \mathcal{N}(y^* | m_{GP}(\mathbf{x}^*), \sigma_{GP}^2(\mathbf{x}^*)) \quad (24)$$

Here,  $y^*$  is the predicted observation for a new input  $x^*$  that is not contained in the training data. Notice  $y^*$  is a random scalar and its predictive distribution is Gaussian with predictive mean  $m_{GP}(\mathbf{x}^*)$  and predictive variance  $\sigma_{GP}^2(\mathbf{x}^*)$  functions:

$$\begin{aligned} m_{GP}(\mathbf{x}^*) &= \mathbf{k}^T \mathbf{C}^{-1} \mathbf{y} \\ \sigma_{GP}^2(\mathbf{x}^*) &= c - \mathbf{k}^T \mathbf{C}^{-1} \mathbf{k} \end{aligned} \quad (25)$$

These functions depend on  $\mathbf{x}^*$  through  $c = k(\mathbf{x}^*, \mathbf{x}^*)$  and  $\mathbf{k} = [k(\mathbf{x}_1, \mathbf{x}^*), \dots, k(\mathbf{x}_N, \mathbf{x}^*)]^T$ .

### 4) Hybrid surrogate model:

As we will see later, there are advantages and disadvantages to both physics-based and data-driven surrogate models. We now consider a Kennedy-O'Hagan hybrid model:

$$\begin{aligned} y_i &= \eta(\mathbf{x}_i, \theta) + \delta(\mathbf{x}_i; \phi) + \epsilon_i, \\ \eta(\mathbf{x}_i, \theta) &= \frac{2v_0^2}{g} \sin(\psi) \cos(\psi) \\ \delta(\mathbf{x}_i; \phi) + \epsilon_i &\sim \mathcal{GP}(\mu(\cdot), k(\cdot, \cdot)) \end{aligned} \quad (26)$$

Here, we combine the simple physics surrogate model Eq. (18) and the data-driven Gaussian process Eqs. (19) - (25) to establish the Bayesian hybrid model Eq. (26). We

note that the GP surrogate is now trained on the difference between the observations  $\mathbf{y}$  and the simple physics model outputs  $\eta(\mathbf{x}, \theta)$ .

### B. Training Data

We assume  $g = 9.8 \text{ m/s}^2$  and  $C_D/m = 0.01 \text{ kg/m}^2$  and simulate the full physics model, Eq. (3) - (16), to generate training data. Each experiment consists of the initial velocity  $v_0$ , firing angle  $\psi$ , and observed impact location  $y$  (horizontal distance traveled). We add Gaussian observation noise with mean zero and standard deviation 5 m to represent aleatoric uncertainty. Figure 1 and Table I summarizes the training data. In this paper, experiments 1-5 act as a base training dataset. We compare the impact of selecting either experiment 6a, 6b, or 6c as the sixth experiment on both Bayesian model calibration and optimization under uncertainty.

TABLE I

TRAINING DATA GENERATED FROM FULL PHYSICS MODEL.

Experiment	Angle ( $^\circ$ )	Initial velocity (m/s)	Impact location (m)
	$\psi$	$v_0$	$y$
1	25	60	118.18
2	30	70	159.79
3	36	80	174.14
4	45	90	181.67
5	60	75	143.21
6a	10	42	47.305
6b	80	53	54.294
6c	85	71	43.239

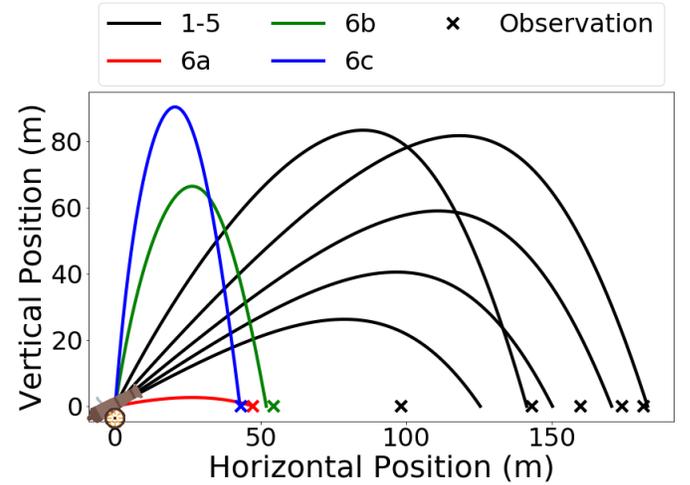


Fig. 1. Trajectories for training data generated from the full physics model. Significant air resistance causes the trajectories to be not parabolic.  $\times$  marks the observed distance traveled and includes observation error.

### C. Bayesian Calibration

For each of the three postulated models, we wish to use a subset of the training data to infer the unknown model parameters. We use a Bayesian approach, i.e., Eq. (2), which takes a prior distribution and computes a posterior distribution. For all three surrogate models, Bayesian calibration is performed using Markov Chain Monte Carlo implemented in Python using the PyMC3 package [30].

1) *Simple physics surrogate model:* In the simple physics model, Eq. (18), we seek to estimate parameter  $g$ . We use a uniform prior distribution:

$$\frac{1}{g} \sim \mathcal{U}(0.001, 1) \quad (27)$$

The likelihood  $p(\mathcal{D}|\omega)$  is assumed to follow a normal distribution. This is equivalent to assuming the observation error is normally distributed.

$$p(\mathcal{D}|\omega) = \mathcal{N}(\eta(\mathbf{x}_i, g), \tau^{-1}) \quad (28)$$

Here,  $\eta(\mathbf{x}_i, g)$  is the simple model and  $\tau$  is the precision, i.e., inverse of the observation error variance. We assume a gamma prior for hyperparameter  $\tau$ :

$$\tau \sim \mathcal{G}(0.25, 2.5) \quad (29)$$

For the simple model, only one model parameter ( $g$ ) and one model hyperparameter ( $\tau$ ) needs to be estimated, thus:

$$\omega = [g, \tau] \quad (30)$$

2) *GP surrogate model:* Recall for the ballistics problem,  $D = 2$ . The hyperparameters  $\phi = [\sigma_f^2, l_1, l_2, \sigma^2]$  includes the kernel variance  $\sigma_f^2$ , length scales  $l_1$  and  $l_2$  and likelihood variance  $\sigma^2$ . The hyperparameters are given the following prior distributions:

$$\begin{aligned} \sigma_f &\sim \mathcal{U}(0.1, 1) \\ l_i &\sim \mathcal{U}(1, 50) \\ \sigma &\sim \mathcal{N}(0, 5) \end{aligned} \quad (31)$$

We combine these prior distributions with the marginal likelihood, Eq. 23, which gives the the unnormalized posterior. We then compute a maximum a posteriori (MAP) point estimate for the four GP hyperparameters:

$$\phi = [\sigma_f^2, l_1, l_2, \sigma^2] \quad (32)$$

With the estimated  $\phi$  and an arbitrary input  $\mathbf{x}^*$ , predictive mean and variance can be calculated by Eq. (25).

3) *Hybrid surrogate model:* Calibrating the hybrid model requires inferring the parameters in both the glass-box and data-driven components. Thus,

$$\theta = g, \quad \phi = [\sigma_f^2, l_1, l_2, \sigma^2] \quad (33)$$

To train this hybrid model, we first infer  $g$  using Bayesian regression. We then compute the residual  $y_i - \eta(\mathbf{x}_i, g)$ . Finally, we train the GP via MAP estimation on the residual with the prior distributions in Eq. (31).

#### D. Optimization under Uncertainty

We now use the posterior distribution from Bayesian calibration for optimization under uncertainty. Specifically, we seek a velocity  $v_0$  and angle  $\psi$  pair to hit a target at  $\bar{y} = 100$  m, which we formulate as a single-stage stochastic program:

$$\max_{v_0, \psi} \mathbb{E}[u(\bar{y} - y_j)], \quad u(\Delta y) = 1 - \frac{1}{100} \min(\Delta y, 100) \quad (34)$$

The utility function  $u(\cdot)$  varies linearly from unity for a direct hit to zero for a miss of 100 meters or more. We approximate the expectation in Eq. (34) using 4500 samples from the posterior distribution of  $\theta$ . For computational simplicity, we use a MAP point estimate for hyperparameters  $\phi$ . For all three surrogate models, we use a Gauss-Hermite quadrature rule with 7 nodes to approximate the expected value from the GP prediction (if applicable) and observation error distributions. We perform optimization by grid search from  $v_0 = 40$  to 100 m/s and  $\psi = 1^\circ$  to  $90^\circ$  to facilitate visualization.

#### E. Results

We now compare the Bayesian calibration and optimization under uncertainty workflow for combinations of three training datasets (A, B, C) and three models (simple physics, GP, hybrid). For each training dataset, we perform Bayesian calibration and then compute  $v_0^\dagger$  and  $\psi^\dagger$  that maximize Eq. (34). Each training dataset has six experiments. The first five experiments are consistent across all training sets. Table II shows how changing the 6th experiment impacts the optimization results. From Table II, we observe several trends:

- 1) The **glass-box simple physics surrogate model** behaves poorly and consistently overshoots the target by at least 39 m each time. This is because the simple model fails to account for all physical phenomena governing projectile motion, specifically, air-resistance effects. The maximum objective value calculated using the simple physics model to find the optimum firing angle and velocity is 0.698. Recall the objective value 1 indicates a direct hit of the target with exact certainty.
- 2) The **black-box GP surrogate model** also consistently misses the target, but the maximum distance overshoot is 32 m which is less than that for e model. The superior performance of the GP model can be attributed to its purely data-driven nature, with no reliance on the physics governing the process. The maximum objective value calculated when using the pure GP model is 0.818.
- 3) The **hybrid surrogate model** outperforms the simple and GP models. Out of the nine model and data set combinations, the maximum overshooting is restricted to 18 m. We attribute the success of the hybrid model to its ability to learn missing physics with less data from the pure data-driven approach. The maximum objective value obtained when using the hybrid model is 0.987.

Next, we examine training dataset C to further compare the models. Figures 2 - 4 show the contours of the objective function in Eq. (34) for all three models. Recall, the utility function  $u(\cdot)$  varies linearly between 1.0 for a direct hit and 0.0 for a miss of 100 m or more. The dashed blue line shows  $\psi, v_0$  combinations for a direct hit with the full physics model, i.e., the truth simulation. We make several observations from these plots:

- 1) In Figure 2 we see wide contours for the objective that peak below 0.7. This indicates that there is high

TABLE II  
RESULTS FOR CALIBRATION AND OPTIMIZATION WITH NINE MODEL AND TRAINING DATASET COMBINATIONS.

Training set	Training experiments	Calibrated model	Optimum angle ( $^\circ$ )	Optimum velocity (m/s)	Expected distance (m)	Observed distance (m)
			$\psi^\dagger$	$v_0^\dagger$	$y$	
A	1,2,3,4,5,6a	Simple	40	60.0	97.0	141
		GP	29	57.5	137	120
		Hybrid	22	57.5	77.7	113
B	1,2,3,4,5,6b	Simple	18	77.5	97.0	139
		GP	31	57.5	138	132
		Hybrid	22	57.5	77.7	118
C	1,2,3,4,5,6c	Simple	13	90.0	96.0	139
		GP	26	60.0	137	118
		Hybrid	72	72.5	97.7	116

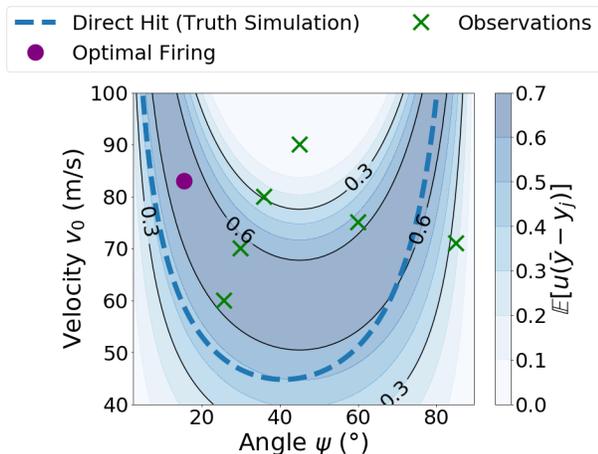


Fig. 2. The wide contours of the objective function  $\mathbb{E}[u]$  indicate high uncertainty using the **simple model**. The highest objective value achieved is 0.698 ( $\mathbb{E}[u] = 1$  indicates a direct hit with probability 1).

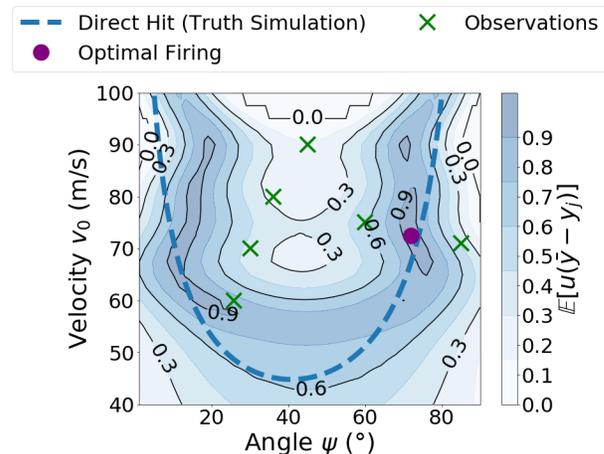


Fig. 4. The **hybrid model** performs the best out of the three models with the highest objective value of 0.987 ( $\mathbb{E}[u] = 1$  indicates a direct hit with probability 1). The physics from the simple model makes the model sensitive to the firing angle and the GP accounts for the neglected air resistance in the simple model to provide the optimal firing conditions.

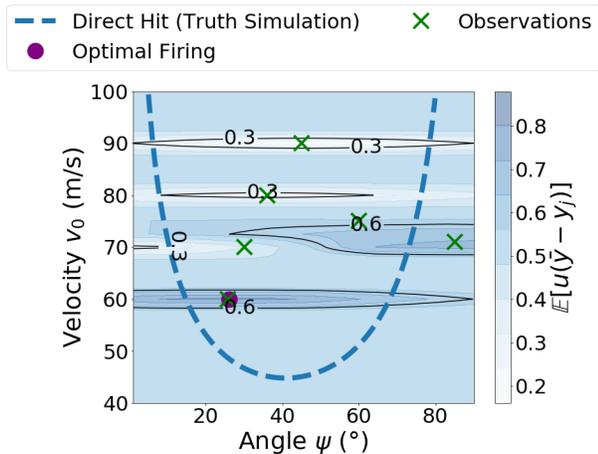


Fig. 3. The narrower contours of the objective function with the **GP model** indicate lower uncertainty than the simple model. The highest objective value calculated is 0.818 ( $\mathbb{E}[u] = 1$  indicates a direct hit with probability 1). The model is insensitive to variations in firing angle indicating the need to refine the training procedure.

uncertainty with the **simple model**. Moreover, the average value for  $g$  in the posterior is  $35.933 \text{ m/s}^2$ . The estimate of  $g$  is biased to offset the missing air resistance in the model.

- 2) While Figure 3 shows higher objective values (above 0.8), it also reveals oblong contours. The **GP model** is fairly insensitive to angle  $\psi$ . This suggests further refinements of the kernel or input transformations or both should be explored.
- 3) Figure 4 illustrates the superior performance of the **hybrid model**. The glass-box component provides the basic shape and the data-driven component corrects for missing physics. As expected, the contours of the hybrid model best align with the truth simulation in regions near training data.

#### IV. CONCLUSIONS

Through the ballistics illustrative example, we compare three surrogate modeling paradigms: glass-box, data-driven, and hybrid. We establish a Bayesian workflow for data-informed decision-making under uncertainty, where the posterior distribution from Bayesian inference is directly used for stochastic programming. We see how model-form uncertainty, specifically neglecting air resistance, biases both parameter estimates ( $g$  is 4 times larger than reality) and predictions (always overshoots). Moreover, the purely data-driven approach using GP regression requires careful tuning

and struggles with limited data. We found the Kennedy-O’Hagan hybrid models overcome limitations of both of these approaches. However, an open question in Bayesian and GP modeling is the judicious selection of training data, kernel functions, and priors. We will explore this and efficient techniques to scale the proposed workflow for higher-dimensional problems in our future work.

More broadly, Kennedy-O’Hagan hybrid models provide a principle approach to quantify epistemic (i.e., model-form) uncertainty in stochastic control and decision-making. We specifically advocate for a Bayesian approach, which provides a rich statistical framework to obtain probability distributions from data that are needed for stochastic programming. We hypothesize that the hybrid model will require orders of magnitude less data than emerging deep-learning black-box models. We plan to rigorously explore this as future work. We also plan to expand the ballistics case study by comparing how each modeling approach performs with additional data. We foresee increasing the size of the training data and exploring transformations will reduce the uncertainty in both GP and hybrid model predictions. We also plan to compare sequential and simultaneous inference of parameters  $\theta$  and hyperparameters  $\phi$ . We hypothesize the latter can reduce bias. We are also interested in other acquisition functions to manage the trade-off between exploration (reducing model uncertainty) and exploitation (direct hit) [18]. Finally, we plan to consider large-scale applications such as chemical reactor kinetic modeling, design, and control.

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