Modeling methods for merging computational and experimental aerodynamic pressure data

Jacob Courtney Haderlie

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By Jacob Courtney Haderlie

Entitled
MODELING METHODS FOR MERGING COMPUTATIONAL AND EXPERIMENTAL AERODYNAMIC PRESSURE DATA

For the degree of Doctor of Philosophy

Is approved by the final examining committee:

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Approved by Major Professor(s): William A. Crossley

Weinong Wayne Chen 12/15/2016
Head of the Departmental Graduate Program Date
MODELING METHODS FOR MERGING COMPUTATIONAL AND EXPERIMENTAL AERODYNAMIC PRESSURE DATA

A Dissertation
Submitted to the Faculty
of
Purdue University
by
Jacob C. Haderlie

In Partial Fulfillment of the Requirements for the Degree of
Doctor of Philosophy

December 2016
Purdue University
West Lafayette, Indiana
To my family
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### ABBREVIATIONS

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<tr>
<td>CFD</td>
<td>Computational fluid dynamics</td>
</tr>
<tr>
<td>DCI</td>
<td>Data-cluster identity</td>
</tr>
<tr>
<td>DOE</td>
<td>Design of experiments</td>
</tr>
<tr>
<td>ECDF</td>
<td>Empirical cumulative density function</td>
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<tr>
<td>GMM</td>
<td>Gaussian mixture model</td>
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<tr>
<td>GP</td>
<td>Gaussian process</td>
</tr>
<tr>
<td>gPoE</td>
<td>Generalized product of experts</td>
</tr>
<tr>
<td>HiLiftPW-1</td>
<td>First AIAA CFD High-Lift Prediction Workshop</td>
</tr>
<tr>
<td>IQR</td>
<td>Interquartile range</td>
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<tr>
<td>MAE</td>
<td>Mean absolute error</td>
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<td>MAP</td>
<td>Maximum a posteriori</td>
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<tr>
<td>Mat</td>
<td>Matérn</td>
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<tr>
<td>MLE</td>
<td>Maximum likelihood estimate</td>
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<tr>
<td>NN</td>
<td>Neural network</td>
</tr>
<tr>
<td>PoE</td>
<td>Product of experts</td>
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<tr>
<td>RMSE</td>
<td>Root mean square error</td>
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<tr>
<td>RQ</td>
<td>Rational quadratic</td>
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<tr>
<td>SEM</td>
<td>Standard error of the mean</td>
</tr>
<tr>
<td>SE</td>
<td>Squared exponential</td>
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<tr>
<td>SVD</td>
<td>Singular value decomposition</td>
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<td>WT</td>
<td>Wind tunnel</td>
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NOMENCLATURE

$B_i^k$  B-spline basis function in the knot interval $i$ of degree $k$

$C_p$  Coefficient of pressure

$C_p$  Additive corrector value

$d$  Number of independent variable dimensions

$f$  Represents actual process in GP model with no $y^m$

$g$  Represents actual process in GP model with $y^m$

$H$  Gaussian process basis function matrix

$k$  Covariance or kernel function

$K$  Matrix of covariance function values

$l$  Gaussian process length scale

$n$  Number of data points

$P$  B-spline control points

$r$  B-spline approximation

$s$  Normalized arc length

$t$  B-spline knot

$w$  Weights

$W_\delta$  Stochastic process, $\mathcal{N}(0, K)$

$x$  Design variable vector

$(x, y, z)$  Wing geometry variables

$y$  Dependent (response) variable vector

$y/b$  Normalized span length

$y^m$  Model basis function in Gaussian process model

$y_{lo}$  Low-fidelity model

$y_{hi}$  High-fidelity model

$\mathcal{D}$  Data set
\( \alpha \)  
Angle of attack

\( \beta \)  
Gaussian process regression parameters

\( \gamma \)  
Gaussian process length scale

\( \delta \)  
Location correction term in Gaussian process basis function

\( \epsilon \)  
Zero-mean Gaussian measurement noise

\( \eta \)  
Normalized span length, \( y/b/2 \)

\( \theta \)  
Gaussian process hyperparameter vector

\( \mu \)  
Mean of the Gaussian process

\( \nu \)  
Gaussian process length scale

\( \rho \)  
Scale correction term in Gaussian process basis function

\( \sigma^2 \)  
Covariance function’s signal variance in Gaussian process model

Subscripts

\( * \)  
Test data locations in the surrogate model

Superscripts

\( (-i) \)  
Data point \( i \) not included in set

\( t \)  
Training data

Diacritical mark

\( (\hat{\cdot}) \)  
Indicates surrogate model
ABSTRACT


Developing the aerodynamic database for aircraft design and analysis depends initially on wind tunnel (WT) testing and computational fluid dynamic (CFD) simulations to describe the pressure nearly anywhere on the surface of an aircraft. This development requires either a significant amount of test data and equipment, a significant increase from current levels in the confidence of computational fluid dynamics, or the merging of computational and experimental data. The cost of experimental testing and the lack of confidence in and/or accuracy of computational results means that merging the computer and wind tunnel data sources seems to be the most probable near-term improvement in developing the aerodynamic database; however, there are no well-established merging methods. Aerodynamic loads engineers, by necessity do perform some kind of merging of CFD results and wind tunnel measurements, but increasing the level of automation and reducing the amount of ad-hoc steps in the current process would provide a significant improvement over the current state of practice. This research describes a process to model surface pressure data sets as a function of wing geometry from computational and wind tunnel sources and then merge them into a single predicted value. The described merging process will enable engineers to integrate these data sets with the goal of utilizing the advantages of each data source while overcoming the limitations of both; this provides a single, combined data set to support analysis and design. The main challenge with this process is accurately representing each data source everywhere on the wing. Additionally, this effort demonstrates methods to model wind tunnel pressure data as a function of angle of attack as an initial step towards a merging process that uses both location on the
wing and flow conditions (e.g., angle of attack, flow velocity or Reynold’s number) as independent variables. This surrogate model of pressure as a function of angle of attack can be useful for engineers that need to predict the location of zero-order discontinuities, e.g., flow separation or normal shocks.

Because, to the author’s best knowledge, there is no published, well-established merging method for aerodynamic pressure data (here, the coefficient of pressure $C_p$), this work identifies promising modeling and merging methods, and then makes a critical comparison of these methods. Surrogate models represent the pressure data for both data sets. Cubic B-spline surrogate models represent the computational simulation results. Machine learning and multi-fidelity surrogate models represent the experimental data. This research compares three surrogates for the experimental data (sequential—a.k.a. online—Gaussian processes, batch Gaussian processes, and multi-fidelity additive corrector) on the merits of accuracy and computational cost. The Gaussian process (GP) methods employ cubic B-spline CFD surrogates as a model basis function to build a surrogate model of the WT data, and this usage of the CFD surrogate in building the WT data could serve as a “merging” because the resulting WT pressure prediction uses information from both sources. In the GP approach, this model basis function concept seems to place more “weight” on the $C_p$ values from the wind tunnel (WT) because the GP surrogate uses the CFD to approximate the WT data values. Conversely, the computationally inexpensive additive corrector method uses the CFD B-spline surrogate to define the shape of the spanwise distribution of the $C_p$ while minimizing prediction error at all spanwise locations for a given arc length position; this, too, combines information from both sources to make a prediction of the 2-D WT-based $C_p$ distribution, but the additive corrector approach gives more weight to the CFD prediction than to the WT data.

Three surrogate models of the experimental data as a function of angle of attack are also compared for accuracy and computational cost. These surrogates are a single Gaussian process model (a single “expert”), product of experts, and generalized product of experts.
The merging approach provides a single pressure distribution that combines experimental and computational data. Results show that sequential Gaussian processes provide better experimental surrogates for pressures at wing locations than batch Gaussian processes or additive corrector surrogates, but at much higher computational cost and lower accuracy away from WT data locations than either of the other methods. The batch Gaussian process method provides a relatively accurate surrogate that is computationally acceptable, and can receive wind tunnel data from port locations that are not necessarily parallel to a variable direction. On the other hand, the sequential Gaussian process and additive corrector methods must receive a sufficient number of data points aligned with one direction, e.g., from pressure port bands (tap rows) aligned with the freestream. The generalized product of experts best represents wind tunnel pressure as a function of angle of attack, but at higher computational cost than the single expert approach. The format of the application data from computational and experimental sources in this work precluded the merging process from including flow condition variables (e.g., angle of attack) in the independent variables, so the merging process is only conducted in the wing geometry variables of arc length and span.

The merging process of $C_p$ data allows a more “hands-off” approach to aircraft design and analysis, (i.e., not as many engineers needed to debate the $C_p$ distribution shape) and generates $C_p$ predictions at any location on the wing. However, the cost with these benefits are engineer time (learning how to build surrogates), computational time in constructing the surrogates, and surrogate accuracy (surrogates introduce error into data predictions). This dissertation effort used the Trap Wing / First AIAA CFD High-Lift Prediction Workshop as a relevant transonic wing with a multi-element high-lift system, and this work identified that the batch GP model for the WT data and the B-spline surrogate for the CFD might best be combined using expert belief weights to describe $C_p$ as a function of location on the wing element surface.
1. INTRODUCTION

1.1 Research Objectives and Motivation

Developing an aerodynamic database for aircraft design and analysis depends initially on wind tunnel (WT) testing and computational fluid dynamic (CFD) simulations. Current issues with each data source are that wind tunnel testing can be costly and time consuming, while confidence in using CFD is slowly increasing. The data sources produce results that do not always agree. Questions asked were:

- is there a process to synergistically combine data from the computational and experimental sources to integrate advantages from each and limit their respective disadvantages?

and

- will this merging process provide a more automated approach to developing the aerodynamic database?

This dissertation demonstrates methods to answer these questions via the merging process and surrogate modeling, identifies promising methods, and assesses which of these methods work best.

The merging process presented here relies on surrogate modeling to represent the experimental and computational coefficient of pressure ($C_p$) data at any point on the wing, not just at data collection locations. This work investigated building $C_p$ surrogate models in wing geometry and angle of attack variables (arc length, span, and angle of attack), but the quantity of computational data in angle of attack did not allow construction of CFD surrogate models in all three dimensions, which consequently, also prohibited WT surrogate model construction in all three dimensions. Thus, the modeling and merging of CFD and WT $C_p$ data occurs in arc length and
span variables, while WT surrogate models are separately generated as a function of only angle of attack. Wind tunnel surrogate models in angle of attack may be helpful in predicting flow discontinuities from physical phenomenon, e.g., flow separation or normal shocks. Surrogate models are approximations of the actual data, which introduces error into the response predictions. But, as John Tukey said, “Far better an approximate answer to the \textit{right} question, \ldots than an \textit{exact} answer to the wrong question” \cite{1}. This research seeks to answer the two “right” questions listed in the previous paragraph. The cost of generating the “approximate answers” (merged $C_p$ distribution predictions using surrogate models) is that the approximate answers introduce error into the final $C_p$ predictions.

Section 1.2 explains the conceptual approach to data merging in this work, Section 1.3 provides a brief explanation of and for using surrogate modeling in this research, and Section 1.4 describes the outline for the rest of the dissertation.

1.2 Merging Process Overview

Developing the aerodynamic database to describe pressure nearly anywhere on the surface of the aircraft requires a significant amount of test instrumentation, a significant increase in confidence of the CFD, or the merging of CFD results and wind tunnel data. Thus, a merging process is presented here as a solution to develop the aerodynamic database. Merging experimental and computational aerodynamic data (In this research, this data is the coefficient of pressure, $C_p$) requires methods that utilize the advantages of each data source while mitigating the limitations of each. The merging process challenges are 1) the lack of collocated output responses, 2) output responses with similar trends, but different values, 3) working with measurement noise from WT observations and deterministic CFD results, 4) modeling large changes in $C_p$ slope and curvature that result from actual flow phenomenon (e.g., large pressure fluctuations near the wing leading edge), and 5) generating a merged data set at low computational cost.
Pressure values from WT experiments are associated with a relatively small number of pressure port (tap) locations, while pressure values from CFD simulations are associated with a computational grid that correspond to a large number of locations on the aircraft surface. In general, generating a merged “field” of pressure information requires collocated information, i.e., obtaining the merged pressure value requires information from CFD and WT data at the same geometric location. Often, different data sets do not provide collocated information. Surrogate modeling can solve the collocated-pressure-information problem (the first merging process challenge in the previous paragraph). Surrogates allow the prediction or representation of response values (e.g., $C_p$) as a function of the independent variables (e.g., arc length or span).

Figure 1.1 overviews the merging process the data merging team conjectured, which relies heavily on surrogate modeling. The merging process in Fig. 1.1 solves challenges two through five mentioned above with surrogate models that can account for each data source’s characteristics, and a merging method combining deterministic and stochastic data. The CFD and WT data sources provide $C_p$ information as a function of independent variables at discrete locations where data is available from either source. The points $x_m$ would describe the arc length and span positions in the CFD grid on the surface, while the points $x_k$ would describe the positions of the pressure ports. Chapter 3 discusses why and how cubic B-spline models and the
tensor-product, i.e., multivariate, B-spline methodology represent the CFD simulation results.

Calibration is often understood to mean improving the accuracy of one system by comparing the results with another system that is certified to be more accurate than the first. However, in this context, calibration of data set $D_1$ (here, WT) using data set $D_2$ (CFD) uses information from $D_2$ to estimate $D_1$ surrogate model parameters that characterize the underlying physics of $D_1$ responses. In other words, the calibration process uses information-rich data sources (CFD results at WT pressure port locations, $\hat{C}_{p,\text{CFD}}(x_k)$) to calibrate the surrogates of information-scarce data sources (WT data) by informing the information-scarce surrogate model of the shape of the data. This does not imply that either data set is of higher or lower fidelity, but leverages information from one data source to improve the surrogate model of another source. This research investigated and evaluated multiple calibration process methodologies illustrated by the flow chart in Fig. 1.2. In general, these methodologies used Gaussian process (GP) regression modeling and an additive corrector approach from the multi-fidelity design and analysis field. Chapters 4 and 5 discuss these surrogate models in detail, respectively.

Figure 1.2.: Calibration process overview for wind tunnel data.
1.3 Brief Introduction to Surrogate Modeling

Surrogate modeling allows representations of response data at any value in the domain of the independent variable(s) despite only having a discrete set of observations, as demonstrated in Figure 1.3. Almost all surrogate models have error in the representation of the actual system response, but it is an inexpensive alternative to generating response predictions at any combination of independent variable values of interest.

There are many types of surrogate models, such as polynomial surfaces, Kriging, artificial neural networks, support vector machines, B-splines, Bezier curves, and Gaussian process models. Investigations into multiple surrogate models to represent coefficient of pressure values, $C_p$, indicated that cubic B-splines provided the best surrogate models for the CFD-predicted $C_p$ distribution. Cubic B-splines were ideal for CFD results in this research because of low computational cost for the large amount of CFD data (large compared with the amount of WT data) and the ability to represent $C_p$ distributions as a function of arc length and span. Gaussian process modeling represented the WT data, because the GP regression surrogates can use the CFD B-spline to inform the shape of the WT data in the wing geometry, account for...
measurement noise, approximate large $C_p$ changes and curvature well, and generally models the WT response adequately despite the sparse amount of data.

1.4 Dissertation Outline

The rest of this dissertation discusses the data merging application using the NASA Trap Wing from the First AIAA CFD High-Lift Prediction Workshop [2] in Chapter 2, the B-spline surrogate models for CFD results in Chapter 3, the Gaussian process surrogate models for WT data in the wing geometry in Chapter 4, the additive corrector surrogate model for WT data in the wing geometry in Chapter 5, a comparison of the WT data surrogates (GP and additive corrector methods) in Chapter 6, methods for merging the CFD and WT surrogates in Chapter 7, surrogate modeling methods for WT data as a function of angle of attack in Chapter 8, and the conclusions in Chapter 9. Each chapter will provide a review of other published work relevant to the topic of the chapter. Non-essential, yet potentially illuminating information, appear in the appendices.
2. DATA APPLICATION AND SETUP

The NASA Trapezoidal Wing configuration and data provide a relevant example for a specific application of the aerodynamic data merging research. Section 2.1 discusses this application example, while Section 2.2 covers general CFD and WT data advantages and limitations, and Section 2.3 explains various error metrics considered in this research for surrogate modeling assessment.

2.1 Aerodynamic Data Merging Application: Trap Wing

The aerodynamic data merging process needed a practical example of a high-lift wing configuration with pressure data. The data needed to be both relevant for engineers analyzing wing pressure data and available from computational and experimental sources. Therefore, the NASA Trapezoidal, or Trap, Wing data from the First AIAA CFD High-Lift Prediction Workshop (HiLiftPW-1) provided a suitable data set for a high-lift configuration. The Trap Wing configuration and flow conditions providing relevance for this merging process application include the multi-element wing with deployed slat and flap at low Mach number ($M = 0.2$). The Trap Wing data characteristics providing relevance included first-order discontinuities in pressure from flow around cove corners from CFD simulation results, closely aligned $C_p$ values between CFD and wind tunnel (WT) sources in some regions, clear discrepancies in $C_p$ values between data sources in other regions (Ref. [3]), measurement noise from WT data, and WT data designated as outliers by NASA professionals. Figure 2.1 shows the Trap Wing slat, spar, and flap wing element cross sections near the wing root. This work only used the Configuration 1 (slat and flap deployed 30 and 25 degrees, respectively) data without brackets from the HiLiftPW-1 workshop to investigate and then demonstrate aspects of the aerodynamic data merging process [2].
The CFD and WT data for this work came from simulations conducted by Tony Sclafani (of The Boeing Company, and provided to the author’s colleagues for this project) for the HiLiftPW-1 workshop and from the workshop website, respectively. The author reduced the number of wing geometry variables for both CFD and WT sources from Cartesian coordinates to normalized arc length and span, \((x, y, z) \rightarrow (s, \eta)\), to reduce the computational time. This research parameterized each wing section’s chord and thickness coordinates into normalized arc length, \((x, z) \rightarrow s \in [0, 1]\) (slat, spar, and flap each have their own normalized arc length). The arc length starts at the lower surface trailing edge \((s = 0)\), wraps around the leading edge, and ends at the upper surface trailing edge \((s = 1)\). The normalized arc length is calculated using

\[
s_i = \frac{s_{i-1} + \sqrt{(x_i - x_{i-1})^2 + (z_i - z_{i-1})^2}}{s_{\text{max}}}, \quad s_1 = 0. \tag{2.1}
\]

The normalized span, \(y \rightarrow y/(b/2) = \eta \in [0, 1]\), is the other geometric independent variable for the half-span model \((b/2 = 85.054 \text{ in})\).
2.2 Data Advantages and Limitations

The wind tunnel experiments measure pressure data at pressure ports from discrete wing locations, which are usually few in number in the wing “geography” due to model construction cost and geometric constraints. With the wind tunnel model built, the cost to measure pressure data at many angles of attack at multiple Mach numbers within the operating range of the wind tunnel is relatively negligible. Therefore, wind tunnel data provides the following advantages for data merging: 1) relative ease to collect data at multiple angles of attack, and 2) valuable realistic data on flight characteristics (subject to wind tunnel corrections) that are only surpassed by expensive flight testing. Sleppy et al. [4] mention additional wind tunnel limitations that The Boeing Company / Commercial Airplanes (BCA) mitigate via “standard testing methods and numerical correction schemes.” General wind tunnel data collection limitations are: 1) the scarcity of data in the wing geometry variables due to the ability to place ports, 2) the range of experiments are limited to the available wind tunnel facilities and their operating capacities, 3) the experiments can produce incorrect measurement readings due to faulty or plugged ports, 4) Reynolds number scaling issues for both the wind tunnel model and flow conditions, and 5) the high cost needed to build the wind tunnel model and run the experiment. In short, wind tunnel experiments do provide relatively realistic data, but collecting the data is expensive and limited in wing geography.

Computational fluid dynamic (CFD) simulations model aircraft geometries and flow conditions using a mesh grid extending from the aircraft surface to the freestream. These simulations calculate a converged solution using fluid flow equations; for example, simple, inviscid Euler, or more complicated Navier-Stokes equations. Advantages of using CFD simulation results include 1) a large number of grid points on the wing geometry to model the flow physics, 2) pressure calculations on the surface of the model in locations where placing and plumbing pressure ports would be difficult or impossible, 3) simulations at many possible flow conditions, 4) results not subject to
measurement noise or faulty ports, and 5) the ability to scale the model to match the flight vehicle. Disadvantages of using CFD simulation results include 1) the large computational and time cost of generating the CFD grid and results at each flow condition, thus reducing the number of CFD simulation runs as a function of flow condition variables, and 2) the modeling error associated with the computational simulation of actual flow physics. In summary, for the aerodynamic data merging, CFD simulation results provide a large amount of deterministic data in wing geometry, but with limited accuracy in some regions, e.g., near the wing tip [3], and large cost for results at multiple flow conditions.

Surrogate modeling needs to take advantage of the large amount of CFD data and accuracy of WT observations, while mitigating potential limitations of CFD simulation inaccuracies and WT data scarcity in wing geometry.

2.3 Surrogate Modeling Error Metrics

A surrogate model is a mathematical approximation of a response to given inputs from independent variables

$$y(x) = \hat{y}(x) + \epsilon$$

where the hat designates \(\hat{y}\) as the surrogate of the data \(y\), and \(\epsilon\) is the surrogate error that the model seeks to minimize. A surrogate is also known as a metamodel; although, Ref. [5] differentiates the two for the purpose of their discussion. Surrogate models are popular tools because they provide computationally inexpensive alternatives to costly experiments or simulations when exploring the design space and optimizing the design [5–15]. As mentioned earlier, some popular surrogate models include Kriging, artificial neural networks, polynomial response surfaces (e.g., quadratic response surfaces), B-splines, support vector machines, partial least squares, and Gaussian process models.

Determining if a surrogate model is an appropriate representation of a data set requires a combination of metrics [16], as well as visual inspection of the model.
predictions and data, where available. Determining the appropriate surrogate model requires some “art” as well as “experimentation” with the surrogate models and the data. As Frost said,

“Choosing the correct regression model is as much a science as it is an art. Statistical methods can help point you in the right direction but ultimately you’ll need to incorporate other considerations” [17].

An error metric indicates the surrogate’s residuals at independent variable values which have both surrogate model predictions and data. Summary error metrics combine the residuals from multiple data points into one value to give an overall performance metric. Example summary error metrics include average, maximum, and predictive-error values, e.g., the $L^2$-norm, the $L^\infty$-norm, and cross-validation error calculations, respectively. Some scientists and engineers hold fast to one or two error metrics, but which metrics are most appropriate is problem dependent, and users should not fixate on one or two specific metrics. For example, some scientists contended that the mean absolute error (MAE) is superior to the root mean square error (RMSE) metric [16, 18]. However, Chai and Draxler [16] discuss and prove that using the RMSE “is more appropriate to represent model performance than the MAE when the error distribution is expected to be Gaussian [emphasis added].” When the error distribution is unknown and may be biased, the standard error of the mean (SEM) should replace the RMSE. These three metrics (RMSE, MAE, and SEM) are averaging error metrics (i.e., take some sort of average of the residuals for all data points). The $L^\infty$-norm (infinity norm) error metric indicates the model’s maximum absolute error.

The RMSE, SEM, MAE, and $L^\infty$-norm error metric equations are presented here for completeness, and used later on in the thesis, e.g. Section 6.2. Table 2.1 lists the error metrics and the corresponding equations for the modeling error $e_i$ at observation $i$, where observation $i$ corresponds to a generic set of independent variable values where both the surrogate model and data source provide predictions and observation values, respectively. The SEM equation is the sample standard deviation divided by
the square root of the number of observations, and $\bar{e}$ in this equation is the average modeling error. Chapters 3, 4, 8, and appendices show figure results using these error metric equations. Chapter 6 also discusses surrogate modeling results with these error metrics.

Table 2.1: Error metric equations

<table>
<thead>
<tr>
<th>Metric</th>
<th>Equation</th>
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<tbody>
<tr>
<td>RMSE</td>
<td>$\sqrt{\frac{1}{n} \sum_{i=1}^{n} e_i^2}$</td>
</tr>
<tr>
<td>MAE</td>
<td>$\frac{1}{n} \sum_{i=1}^{n}</td>
</tr>
<tr>
<td>SEM</td>
<td>$\sqrt{\frac{1}{n} \sum_{i=1}^{n} (e_i - \bar{e})^2}$</td>
</tr>
<tr>
<td>$L^\infty$-norm</td>
<td>$\max{</td>
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</table>
3. **B-SPLINE SURROGATE MODELS**

Selecting the best surrogate to represent the CFD simulation results turned out to be part art and part science [17]. The initial test model was a simple wing geometry with a constant NACA 0021 airfoil section, no sweep, no dihedral, and no taper (rectangular wing). XFLR5 (a panel code of three-dimensional wing geometry) and CFD using Reynolds-averaged Navier-Stokes (RANS) equations provided the first set of test data. Initial surrogate model investigations of the CFD $C_p$ distributions compared linear interpolation, Kriging (a Gaussian process model with a specific covariance function), and B-spline models on a simple wing (rectangular wing with no sweep or dihedral and a constant NACA 0021 airfoil section). The cubic B-spline model produced surrogates with lower error and greater predictive capability than the linear interpolation or Kriging models. This work found that a tensor product B-spline best represents the CFD-generated surface $C_p$ data with cubic B-splines in geometric dimensions $(s, \eta)$. B-splines are used because of the low computational cost as well as the ability to approximate arbitrary pressure distributions in the arc length and spanwise directions. Carl de Boor published the seminal work on B-splines [19]. Cheney and Kincaid published another good resource [20]. The discussion that follows here presents the important features of B-splines in a context relevant to the aerodynamic data merging process.

3.1 **Basis functions and control points**

B-spline approximations are built using basis functions and control points specified by knot locations, $t$, the degree of the B-spline, $k$, and the output response at
independent variable values, \( y(x) \). The B-spline basis functions require a zero degree (first order) anchor

\[
B_i^0(x) = \begin{cases} 
1 & t_i \leq x \leq t_{i+1} \\
0 & \text{otherwise}
\end{cases}. \quad (3.1)
\]

Using \( B_i^0 \) as the anchor, the higher-order B-spline basis functions from Carl de Boor’s recursive formula are [20]

\[
B_i^k(x) = \frac{x-t_i}{t_{i+k}-t_i} B_{i}^{k-1}(x) + \frac{t_{i+k+1}-x}{t_{i+k+1}-t_{i+1}} B_{i+1}^{k-1}(x), \quad k > 0. \quad (3.2)
\]

The superscript and subscript values are the degree of the basis function \( k = 1, 2, \ldots \) and the knot interval \( i = 0, \pm 1, \pm 2, \ldots \). Figure 3.1 illustrates B-spline basis functions from zero to three degrees for evenly spaced knots on the interval \( x \in [0, 1] \). Cubic B-spline basis functions \((k = 3)\) are used in this work because of their smoothness, and their ability to represent arbitrary pressure distributions well. See Ref. [20] for more discussion on basis functions and illustrations.

B-spline surrogates need a large number of knots in some locations to represent abrupt changes in values of the data the B-spline is intending to represent. Increasing the number of knots allows for more curvature changes in the approximation,
but this also increases the computational cost to solve for the control points needed to build the B-spline. Knots are placed at dyadic intervals (i.e., a new knot is placed at the midpoint between other knots) for tensor product B-splines, which minimizes the number of overall knots in each dimension. This knot placement methodology is discussed in detail in Section 3.2.

The control points are calculated, after generating the B-spline basis functions of degree $k$, using the following formula

$$\mathbf{P}(\mathbf{x}) = (B^k(\mathbf{x}))^{-1} \mathbf{y}(\mathbf{x})$$

(3.3)

where $\mathbf{y}$ is the data response vector (in this work, this response vector is a one-dimensional set of $C_p$ data from the CFD simulation results, $\mathbf{y}(\mathbf{x}) = C_{p,CFD}(\mathbf{x})$).

With the knot locations and B-spline degree defined, the basis functions and control points are easily calculated, from which the B-spline surrogate is calculated using

$$\mathbf{r}(\mathbf{x}) = \sum_{i=0}^{m} \mathbf{P}_i(\mathbf{x}) B^k_i(\mathbf{x})$$

(3.4)

where $\mathbf{r}$ is the B-spline approximation for $m + 1$ knot intervals. Thus, the only ways to improve the B-spline surrogate approximation are through increasing the number of knots or changing the B-spline degree. Cubic B-splines are commonly used in generating approximations, so only the number of knots are changed here to improve the surrogate modeling accuracy. The above B-spline approximation formula is for a one-dimensional (1-D) approximation, and this work needed a 2-D approximation of the CFD $C_p(s, \eta)$.

Going from 1-D to multivariate B-splines greatly influences the knot placement strategy. So, first the multivariate B-spline is defined, and then the knot location placement strategy is defined.

### 3.2 Multivariate B-splines

Building the multivariate, or tensor product, B-spline surrogate model requires building 1-D B-splines sequentially in each variable direction using a knot-adding
algorithm. The tensor product B-spline requires the user to preprocess the data to ensure that all the data is in an orthogonal grid format. In other words, with the aerodynamic data, each airfoil section data needed to be at constant spanwise values; airfoil sections with multiple $\eta$ values resulted in computational errors. The CFD simulation grid for the NASA Trap Wing aligned with the wing elements’ geometries with the slat and flap stowed, and therefore, when the slat and flap were deployed, the computational grids that did not have constant $\eta$ values. The $C_p$ values are calculated for the orthogonal grid using a bi-linear interpolation from the original arc length and span locations. The process to building the tensor product B-spline is enumerated here, and the corresponding pseudo-code is in Appendix A.

1. Build 1-D B-spline of $C_p$ at each spanwise station, $\eta_j$, using knot-adding algorithm at each station to determine how many knots each airfoil section needs to describe $C_{p,CFD}(s, \eta_j)$
   
   (a) Add knot to domain midpoint, $s = 0.5$ for $s \in [0, 1]$

   (b) Calculate error metric for each knot interval (this work used the $L^2$-norm metric)

   (c) Continue adding knots, $t_s$, to intervals with the largest approximation error until the error-termination criterion is met

      i. Add knots to dyadic intervals (midpoint between knots), e.g., $s = 1/2$, then $1/4$ or $3/4$, then $1/8$, $3/8$, $5/8$, or $7/8$, etc.

2. Calculate the union of knots at each span, $\eta_j$, to get $T_{\eta}$

3. Build 1-D B-spline of $C_p$ at each $\eta_j$ to calculate control points, $P_s$

4. Build 1-D B-spline to $P_s$ (instead of $C_p$) values in spanwise direction at each arc length station, $s_i$ where there are $P_s$ coefficients

5. Perform knot-adding algorithm

6. Take union of knots at each $s_i$ to get $T_s$
7. Build 1-D B-spline of $P_s$ at each $s_i$ to calculate control points, $P_{s,\eta}$

So, building the tensor product B-spline generates a set of knots and 1-D B-spline basis functions from Eq. (3.2) in each variable direction and one $n$-dimensional set of control points for $n$ variables. The 1-D B-spline approximations to the second, third, or higher dimensions are surrogates of the previous dimension's control points, not the data itself.

The resulting multivariate B-spline surrogate model from the above process is of the form

$$
\mathbf{r}(\mathbf{x}, \mathbf{z}) = \sum_{j=0}^{p} B_j^q(\mathbf{z}) \left[ \sum_{i=0}^{m} P_{i,j}(\mathbf{x}, \mathbf{z}) B_i^k(\mathbf{x}) \right]
$$

(3.5)

where the B-spline basis functions for independent variable vectors $\mathbf{x}$ and $\mathbf{z}$ (corresponding to $s$ and $\eta$) are of order $k+1$ and $q+1$ with $m+1$ and $p+1$ knots intervals, respectively. For this application, the $m$ and $p$ knots are for the arc length and span-wise dimensions, respectively. The research effort represented CFD-generated results with a tensor product cubic B-spline in both dimensions, i.e., $k = q = 3$. As a result, the surrogate model of the CFD-generated $C\rho$ values takes the form

$$
\hat{C}_{p,\text{CFD}}(s, \eta) = \sum_{j=0}^{p} B_j^3(\eta) \left[ \sum_{i=0}^{m} P_{i,j}(s, \eta) B_i^3(s) \right].
$$

(3.6)

Each flow condition (each angle of attack) has two sets of knots for arc length and span variables and one multivariate control point array for the cubic B-splines describing the CFD simulation results.

### 3.3 Building and Assessing B-splines for CFD $C\rho$ Distribution

This section demonstrates CFD cubic B-spline surrogate modeling results as well as surrogate error results.
3.3.1 CFD B-spline

The CFD simulation results for the NASA Trap Wing at lower angles of attack (below flow separation at $\alpha \approx 36^\circ$) had very smooth $C_p$ predictions over most of the multi-element wing surface, with the exception of near zero-order discontinuous geometric features, e.g., slat cove corner, or trailing edge. The slat and spar in Fig. 3.2 each have cove corners that generate large pressure spikes over a very small region of the arc length. Figure 3.3 illustrates the slat $C_p$ spike near $s = 0.4$, and contains the entire CFD slat pressure distribution (from inboard to wing tip) simulation results for $\alpha = 6^\circ$. The pressure spike for the slat does not stay at a constant arc length location, but moves from around $s = 0.4$ to about $s = 0.37$. This movement is an artifact of the slat’s changing chord length from inboard to wing tip, and hence the normalized arc length value at the cove corner changes as well. Subject matter experts from Boeing Commercial Airplanes (BCA) Flight Sciences, Loads & Dynamics group

![Figure 3.2: NASA Trap Wing slat, spar, and flap airfoils at $\eta = 0.08$.](image)
suggested that this research did not need to model the pressure spike around slat and spar cove corners, so that data was used in generating the CFD B-spline surrogates. Fewer knots were required to represent CFD $C_p$ data without the $C_p$ spike in the cove corners, which resulted in lower computational cost. This will be evident in the error assessment in Section 3.3.2. Additionally, the transformation of $(x, y, z) \rightarrow (s, \eta)$, as mentioned in Section 2.1, “unwraps” the airfoil so that $s$ starts at the lower surface trailing, wraps around the leading edge, and ends ($s = 1$) at the upper surface trailing edge for each wing element.

Figure 3.4 displays the CFD B-spline pressure distribution predicted values for the Trap Wing flap at $\alpha = 6$ degrees. The color scheme corresponds to the $C_p$ value, and is different from that of Fig. 3.3 to distinguish CFD data from B-spline surrogates. There are four dark bands at constant $\eta$ values that correspond to an increased number of grid points that were used to model support brackets for some portions of the High Lift Prediction Workshop [2]. The pressure distribution is very even over the entire wing until close to the wing tip. Various CFD codes had trouble predicting the pressure at the wing tip for this Trap Wing geometry [3].

Figures 3.3, 3.5, and 3.6 show that the slat and spar CFD data and B-spline $C_p$ distribution predictions at $\alpha = 6$ degrees have more variations than the flap in the
arc length direction, but are relatively smooth in the span direction, until the wing tip. The slat and spar have more disturbances in the arc length direction because of the cove region \((s \in [0, 0.4] \text{ and } [0, 0.1] \text{ for the slat and spar, respectively})\). The slat and spar cove regions have three sharp corners, one at the wing element trailing edge, second near the midpoint of the cove, and the last at the boundary of the cove and “exposed” regions. These sharp corners contribute to larger variations in \(C_p\) distribution than those demonstrated in Fig. 3.4 for the flap on the lower surface near
the trailing edge. Figures 3.3 and 3.7 show the results of the cove corner pressure spike for the slat CFD $C_p$ simulation result values near $s \approx 0.4$ at the boundary or corner of the cove and exposed regions; once again, these figures use a different color map to indicate these are values of $C_p$ predicted by the CFD results, not the B-spline surrogate representation. For this research effort, B-spline surrogates did not model the cove corner spike because of input from subject matter experts, so it is not evident in Figs. 3.5 or 3.6. The CFD simulation results indicate that the spar has an additional flow disturbance from the trailing edge of the slat being right above the spar’s upper surface leading edge, see the wing geometry in Fig. 3.2. This flow disturbance on the spar near the leading edge ($s \approx 0.55$ in Fig. 3.6) causes what appears to be two $C_p$ pressure rises at the leading edge. Wing tip vortices impinging on downstream wing elements create larger pressure rises near the wing tip ($y/b/2$ or $\eta \approx 1$) on the spar and flap compared with those of the slat.
The cubic B-spline surrogate modeling approach captures, at least qualitatively, the pressure distribution—including unusual or abrupt changes in $C_p$ level related to the multi-element wing.

### 3.3.2 CFD B-spline Assessment

The results here document the quantitative assessment of multivariate cubic B-splines representing CFD results using error metrics.

As described in Section 3.2, the two-dimensional (2-D) B-spline approach adds knots using dyadic intervals with the intent of balancing computational effort with providing an acceptably accurate representation of the CFD-generated $C_p$ values. The CFD B-spline surrogates required user-developed and user-specified stopping criteria for placing knots in both arc length and span directions. The algorithm stopped adding knots when the $L^2$-norm of the error between the cubic B-spline surrogate and the CFD-generated $C_p$ values for each knot interval was lower than a user-specified maximum, $(L^2\text{-norm})_{\text{max}}$. The author investigated using maximum and average error metrics with the $L^\infty$-norm and $L^2$-norm metrics, respectively. For this application,
the $L^2$-norm generated quality surrogates with consistency and accuracy than the $L^\infty$-norm.

Figures 3.8 and 3.9 display the absolute difference between the B-spline surrogate and the CFD-computed $C_p$ values on the flap and spar elements of the Trap Wing.

Figure 3.8.: Flap CFD $C_p$ B-spline error at $\alpha = 6^\circ$.

Figure 3.9.: Flap CFD $C_p$ B-spline error at $\alpha = 6^\circ$.

These plots display the generally oscillatory behavior of the error as a function of arc length. The error does not oscillate in span because the $C_p$ distribution does not vary as much in $\eta$ as it does in $s$ (see Fig. 3.4). The error oscillates with respect to arc
length because the multivariate B-spline surrogate will approximate data with error oscillation frequencies proportional to the number of knots in a region. For example, the error oscillations in Fig. 3.9a (profile views of Fig. 3.8) increase in frequency near the flap leading edge ($s \approx 0.5$) because there are significantly more knots placed near the leading edge so the B-spline can model the large changes in curvature in this region because of the pressure rise. Likewise, the oscillation frequency is much lower on the upper and lower surfaces in between the leading and trailing edges ($s \in [0.1, 0.4]$ and $s \in [0.6, 0.9]$). The $C_p$ error magnitude is generally between $[-0.02, 0.02]$, and the maximum error range is very good at 1.14 percent of the maximum flap $C_p$ range for this angle of attack ($C_p$ range of 5.33).

Fig. 3.10 shows the RMSE and MAE for the CFD B-spline surrogates of the flap at a low and a high angle of attack, $\alpha = [6^\circ, 36^\circ]$, respectively (see Table 2.1 for the error metric equations). These error metrics indicate the B-spline surrogate’s high degree of accuracy in predicting the CFD flap pressure distributions. The RMSE and MAE values are higher near the leading edge ($s \approx 0.5$) than other regions because of the large pressure rise near the leading edge (Figs. 3.10a and 3.10c). Figures 3.10b and 3.10d illustrate the higher variability in pressure near the body pod-wing joint ($\eta \approx 0.08$) and at the wing tip ($\eta \approx 1$).

Table 3.1 enumerates overall B-spline error metrics for each wing element at various angles of attack. The RMSE and SEM errors are not identical for any wing element at any angle of attack. These values indicate biased error distributions, and validate the statement by Chai et al. that “the standard error (SE) is equivalent to the RMSE as the sample mean is assumed to be zero [for unbiased error distributions]. For an unknown error distribution, the SE of mean is the square root of the ‘bias-corrected sample variance’ ” [16] (Note that the standard error in Ref. [16] is the same as the standard error of the mean (SEM) defined in Table 2.1, but this work uses SEM so as not to be confused with the squared exponential abbreviation discussed in Chapter 4.). While the errors between the B-spline surrogate and the CFD predictions are small, which leads to reasonably high confidence for using this surrogate.
in a merging process, the errors do exhibit distinct patterns and are, therefore, not random errors [21]. Knot locations determine the B-spline surrogate’s flexibility—more knots in a given region lead to greater surrogate flexibility—and these knots create patterns in the errors as a function of the dependent variables (s and η). This correlated error, while present, does not cause an impediment to using B-splines for this application.

The $L^\infty$-norm (maximum absolute residual) values are quite low for the all surrogates, with magnitudes on the order of $\frac{1}{10}$ to $\frac{1}{100}$. As mentioned earlier, modeling the cove corner $C_p$ jump predicted by CFD simulations (see Fig. 3.3) was not important; therefore, the $C_p$ values around the cove corners were not used in building the
Table 3.1: CFD $C_p$ B-spline errors

<table>
<thead>
<tr>
<th></th>
<th>Metric</th>
<th>6°</th>
<th>13°</th>
<th>21°</th>
<th>34°</th>
<th>37°</th>
</tr>
</thead>
<tbody>
<tr>
<td>Slat</td>
<td>RMSE</td>
<td>0.0051</td>
<td>0.0063</td>
<td>0.0032</td>
<td>0.0075</td>
<td>0.0051</td>
</tr>
<tr>
<td></td>
<td>SEM</td>
<td>$1.4\times10^{-5}$</td>
<td>$1.8\times10^{-5}$</td>
<td>$8.9\times10^{-6}$</td>
<td>$2.1\times10^{-5}$</td>
<td>$1.4\times10^{-5}$</td>
</tr>
<tr>
<td></td>
<td>MAE</td>
<td>0.0031</td>
<td>0.0038</td>
<td>0.0017</td>
<td>0.0032</td>
<td>0.0021</td>
</tr>
<tr>
<td></td>
<td>$L^\infty$-norm</td>
<td>0.0515</td>
<td>0.0569</td>
<td>0.0446</td>
<td>0.1595</td>
<td>0.0710</td>
</tr>
<tr>
<td>Spar</td>
<td>RMSE</td>
<td>0.0033</td>
<td>0.0038</td>
<td>0.0043</td>
<td>0.0038</td>
<td>0.0041</td>
</tr>
<tr>
<td></td>
<td>SEM</td>
<td>$9.8\times10^{-6}$</td>
<td>$1.1\times10^{-5}$</td>
<td>$1.3\times10^{-5}$</td>
<td>$1.1\times10^{-5}$</td>
<td>$1.2\times10^{-5}$</td>
</tr>
<tr>
<td></td>
<td>MAE</td>
<td>0.0016</td>
<td>0.0018</td>
<td>0.0023</td>
<td>0.0019</td>
<td>0.0023</td>
</tr>
<tr>
<td></td>
<td>$L^\infty$-norm</td>
<td>0.1051</td>
<td>0.1246</td>
<td>0.1026</td>
<td>0.0766</td>
<td>0.0587</td>
</tr>
<tr>
<td>Flap</td>
<td>RMSE</td>
<td>0.0032</td>
<td>0.0029</td>
<td>0.0026</td>
<td>0.0031</td>
<td>0.0033</td>
</tr>
<tr>
<td></td>
<td>SEM</td>
<td>$1.1\times10^{-5}$</td>
<td>$1.0\times10^{-5}$</td>
<td>$9.0\times10^{-6}$</td>
<td>$1.1\times10^{-5}$</td>
<td>$1.2\times10^{-5}$</td>
</tr>
<tr>
<td></td>
<td>MAE</td>
<td>0.0019</td>
<td>0.0017</td>
<td>0.0014</td>
<td>0.0019</td>
<td>0.0021</td>
</tr>
<tr>
<td></td>
<td>$L^\infty$-norm</td>
<td>0.0354</td>
<td>0.0289</td>
<td>0.0327</td>
<td>0.0391</td>
<td>0.0373</td>
</tr>
</tbody>
</table>

B-spline surrogate models so that the knot-adding algorithm would not approximate the $C_p$ jumps at the corners. So, the error metrics in Table 3.1 do not account for the residuals between the CFD results and B-spline predictions around the cove corners. Figures 3.11, 3.12, and 3.13 show residuals at the locations used to generate the B-spline surrogates; hence, not near the cove corner locations at $s \approx 0.4$ and 0.1 for the slat and spar, respectively. The B-spline surrogate produces acceptable residuals for the slat, spar, and flap, which are all on the same order of magnitude, regardless of the smoothness of the CFD data.

In conclusion, this chapter demonstrates that a 2-D cubic B-spline with the sequential dyadic knot addition is an acceptable way to represent computational $C_p$ distributions for each wing element of a multi-element wing. The results and error measures support this conclusion. The B-spline surrogate represents CFD pressure distribution better than linear interpolation or Kriging surrogates. The issues with
B-splines are that the errors appear to be non-random and that the cove-corner discontinuity must be left out of the CFD results in order to build a useful B-spline that represents the $C_p$ over the remaining wing element surfaces. This chapter also docu-
ments the methodology the author used to build the cubic B-splines of computational pressure data for both a simplistic wing geometry (rectangular wing with constant airfoil section, no sweep, and no dihedral) as well as the NASA Trap Wing.
4. GAUSSIAN PROCESS REGRESSION MODELS

For the aerodynamic merging process, data from both sources of $C_p$ values require surrogate models so that the process can provide a merged $C_p$ value at any location on the wing surface. While the 2-D cubic B-spline provided the best surrogate for the CFD calculated $C_p$ distribution, the $C_p$ distribution associated with the wind tunnel data required a different surrogate model in large part due to the sparse nature of the data with respect to the spanwise dimension of the wing. The NASA Trap Wing used in this study has only nine pressure port bands common to all wing elements, so there are only nine discrete $\eta$ locations where the wind tunnel measures pressure. The author attempted to use cubic B-splines and polynomial response surfaces, but they could not account for the noisy wind tunnel measurements and / or abrupt changes in the pressure distribution (e.g., near the leading edge, or wing tip). After attempting polynomial response surfaces and cubic B-splines as potential surrogates for the wind tunnel data, the best choice for representing the wind tunnel data is an approach that can use both measured data and also incorporate some other source of information that could make up for the sparseness in the $\eta$ dimension. Some version of a Gaussian Process (GP) regression model appears to be the best option as a surrogate for the wind tunnel data.

A Gaussian process (GP) is a probabilistic distribution over functions. GP regression methods seek to represent an unknown real process, or function, $f$, via supervised learning, i.e., using data responses, $y$, at independent variable input locations, $x$, to estimate model hyperparameters [22–26]. GP model hyperparameters are constants that are usually estimated through either Bayesian inference or maximum likelihood estimation [27], and Section 4.1.1 goes over this estimation process in more detail.
This type of learning is common to surrogate regression modeling. The observation equation is

\[ y(x) = f(x) + \epsilon. \] (4.1)

This observation function has the same basic form as Eq. (2.2) for general surrogate models. In the context of Gaussian processes, the actual function \( f(x) \) and the observations, \( y(x) \) differ by additive noise, \( \epsilon \), which is assumed to follow a Gaussian (or normal) distribution so that \( \epsilon \sim \mathcal{N}(0, \sigma^2) \). The data set \( D^t = \{x^t, y^t\} \) is the training data; i.e., this is the data the GP model uses to estimate the GP parameters that describe the function, \( f \). In general, the GP regression model includes a regression function and a stochastic, or random, process function. The regression function globally approximates the function to be modeled and the random process makes local deviations to fit the surface of the data. The research here focuses on GP regression to generate surrogate models of the experimental observations to represent the pressure data, \( C_p \).

The theory behind GP modeling started at least as far back as with the works of Kolmogorov in 1941 [28] and Wiener in 1949 [29]. In 1973, Matheron [30] formalized the GP prediction in the geostatistics field, where it is perhaps more widely known as kriging after Danie Krige [7,31,32]. Jones et al. [32] provide an excellent introduction to kriging surrogate models, which are GP regression models with a specific covariance function (to be described in Section 4.3). GP methods grew into other fields; in 1989, Sacks et al. [33] reviewed the material in the context of computer experiments. Recent applications of GPs include Kennedy and O’Hagan’s [34] general GP model that calibrate a computational GP model using physical and expert data sources to estimate the model hyperparameters. The GP regression modeling in this research, on the other hand, calibrates the physical (i.e., experimental or wind tunnel) data’s surrogate model using the computational data, as explained in Section 1.2. Reese et al. [35] also calibrate the physical data with computer simulation results and expert opinion “to improve estimation and prediction of the physical process.” However, to
the author’s best knowledge, no process exists that generates surrogate models of the field of pressure distribution as a function of wing design variables.

The rest of this chapter includes a GP mathematical introduction (Section 4.1), a discussion of some GP basis functions (Section 4.2), a discussion of covariance (i.e., kernel) functions and their impact on the GP model (Section 4.3), and a presentation of the modeling results (Section 4.4).

4.1 Mathematical Introduction

From Ref. [23], the formal GP definition is:

**Definition 4.1.1** A Gaussian process is a collection of random variables, any finite number of which have a joint Gaussian distribution.

The process function $f(x)$ in Eq. (4.1) is represented by a GP with mean function vector $\mu(x)$ and covariance function matrix $K(x, x')$ in the following manner

$$f(x) \sim GP(\mu(x), K(x, x'))$$

where,

$$\mu(x) = \mathbb{E}[f(x)]$$

$$K(x, x') = \mathbb{E}[(f(x) - \mu(x))(f(x') - \mu(x'))].$$

The covariance function indicates how the two sets of variable values $x$ and $x'$ change relative to each other. This work assumes a mean function value of zero for $f$, which makes the computations easy. However, the aerodynamic pressure data does not have a zero mean, so Section 4.2 introduces an alternative mean function from Section 2.7 of Ref. [23].

Since the values of the process function $f$ are unknown (assume $f$ is the vector of values for the function $f$), the GP model integrates, or marginalizes out those function values using the marginal likelihood [23]

$$p(y|x) = \int p(y|f, x)p(f|x)df.$$ (4.5)
Here, $p(y|f, x)$ is the likelihood function and $p(f|x)$ is the prior function. The prior is the distribution of process values $f$ given variable values $x$, and the likelihood is the distribution of observed data $y$ given the process and variable values. Thus, the resulting marginal likelihood only requires output response values for specified independent variable inputs. In the aerodynamic data merging context, the wind tunnel pressure measurements at pressure port arc length and span locations are the output responses observations for given inputs, $C_{p,WT}(s, \eta) = y(x)$. So, the marginal likelihood is the probability of observing $C_p$ values given locations $s$ and $\eta$; this is also called the model evidence.

In order to use a GP model as a surrogate, some sort of assumption or choice specifies the prior probability distribution. Here, the prior is a Gaussian, or normal, distribution of the form

$$p(f|x) = N(f|0, K) = (2\pi)^{-\frac{n}{2}} |K|^{-\frac{1}{2}} \exp \left( -\frac{f^T K^{-1} f}{2} \right)$$  \hspace{1cm} (4.6)$$

where $n$ represents the number of observations, and the covariance function at the training locations is abbreviated as $K = K(x, x')$. The experimental data in Eq. (4.1) is assumed to have a noisy Gaussian distribution about the process values with a constant noise variance $\sigma^2_e$

$$p(y|f, x) = N(y|f, \sigma^2_e I) = \frac{(2\pi)^{-\frac{n}{2}}}{\sigma_e} \exp \left( -\frac{(y - f)^T (y - f)}{2\sigma^2_e} \right).$$  \hspace{1cm} (4.7)$$

Therefore, the marginal likelihood, or model evidence, from Eq. (4.5), after substituting in Eqs. (4.6) and (4.7), is

$$p(y|x) = N(y|0, M) = (2\pi)^{-\frac{n}{2}} |M|^{-\frac{1}{2}} \exp \left( -\frac{y^T M^{-1} y}{2} \right)$$  \hspace{1cm} (4.8)$$

with $M = K + \sigma^2_e I$. In this form, the left-hand side $p(y|x)$ represents the probability of the observations $y$ given $x$. Again in the context of aerodynamic merging, this
would represent the probability of the measured values of \( C_p \) given the locations on the surface of the wing; this is the wind tunnel \( C_p \) data. However, to use this idea so that the right-hand side of the equation could provide a surrogate to represent the wind-tunnel measured \( C_p \) distribution, there are several unknown values.

The unknowns are the noise variance constant, \( \sigma^2 \), and the parameters that define the characteristics of the covariance function matrix \( K \). There are multiple forms or approaches to posing the covariance matrix function. For illustration here, if the GP model uses a squared exponential (SE) covariance function,

\[
K(x, x') = \text{cov}(f(x), f(x')) = \sigma_{SE}^2 \exp \left( -\frac{(x - x')^2}{2l^2} \right)
\]

(4.9)

in the prior distribution, the unknowns in \( K \) are \( \sigma_{SE}^2 \) and \( l \). Therefore, the vector of unknown GP model hyperparameters, \( \theta = \{\sigma^2, \sigma_{SE}^2, l\}^\top \), where \( \sigma^2 \), \( \sigma_{SE}^2 \), and \( l \) are the noise variance, the SE signal variance, and the SE length-scale parameter, respectively. The terms kernel and kernel function also refer to the covariance function when discussing Gaussian process models; this dissertation uses these terms interchangeably.

The next step to using a GP model as a surrogate model is to find values for the hyperparameters based upon the observed values of \( y \) taken at corresponding values of \( x \). For aerodynamic merging, this would be finding hyperparameter values so that the GP model’s prediction of \( C_p \) closely matches the measured \( C_p \) values from the wind tunnel at the pressure port locations on the wind tunnel model.

### 4.1.1 Parameter Estimation and Predictive Equations

Gaussian process regression models require hyperparameter estimation, “a non-trivial task” [36]. Indeed, this is the most computationally intensive portion of generating GP models. Bayesian inference and maximum likelihood estimation (MLE) are two methods that can generate GP model hyperparameter estimates. Bayarri
et al. [27] state that, “the full Bayesian analysis is theoretically superior [to MLE], because the resulting variance [in the estimated hyperparameter distribution] takes into account the uncertainty in the” GP model hyperparameters, while the maximum likelihood method only produces single-point estimates; i.e., maximum likelihood does not produce hyperparameter variance estimates.

Hyperparameter distribution estimates from Bayesian analysis allow the user to 1) generate uncertainty estimates about the data predictions, 2) combine the data predictions with uncertainties from multiple sources into one data prediction [37], 3) know how confident the user can be in a mean hyperparameter value (e.g., low variance), and 4) know the distribution of the hyperparameters (e.g., multimodal, normal, lognormal, ...).

Maximizing the log marginal likelihood generates single-point estimates of the GP model hyperparameters, thus uncertainty bounds only reflect uncertainty in the mean prediction, and cannot account for uncertainty in the WT data or model hyperparameters. Despite the disadvantage of only generating point estimates of the parameters, MLEs have a computational savings advantage over the full Bayesian analysis and, for this project, produced similar GP mean predictions with results produced by another researcher on this project using Bayesian inference. Therefore, this research estimated the hyperparameters via the MLE approach.

To determine the hyperparameters using the MLE approach, the idea is to find the set of values $\theta$ that minimizes the negative logarithm of the marginal likelihood, or

$$\hat{\theta} = \arg \min_{\theta} -\log p(y|x). \quad (4.10)$$

The log marginal likelihood (found by taking the logarithm of Eq. (4.8)) is

$$\log p(y|x) = -\frac{1}{2} \left[ n \log 2\pi + \log |M| + y^T M^{-1} y \right]. \quad (4.11)$$

These estimated hyperparameter values $\hat{\theta}$ allow response GP predictions of the process function values at test points, $f(x_\ast)$. For the aerodynamic data merging appli-
cation in this work, the test points correspond to the locations of the pressure ports on the Trap Wing.

The predictive equations for the GP regression model of the process function in Eq. (4.1) at the test points are

$$\tilde{f}_s = K_* M^{-1} y$$

(4.12)

$$\text{cov}(f_s) = K_{ss} - K_* M^{-1} K_*^T.$$  \hspace{1cm} (4.13)

The covariance functions at test locations and the cross-covariance function between training and test locations are $K_{ss} = K(x_s, x_s)$ and $K_* = K(x_s, x)$, respectively. Similarly, the process at test locations is $f_s = f(x_s)$, and the predicted mean values of the process is $\tilde{f}_s$. For aerodynamic data merging, the mean predictions $\tilde{f}_s$ are wind tunnel pressure predictions at test locations $\hat{C}_{p,WT}(s_*^i, \eta_*^i)$. As a reminder when using MLE estimated model hyperparameters, the uncertainty predictions in Eq. (4.13) are only uncertainty bounds in the mean predictions in Eq. (4.12), but do not account for uncertainty in the observation data $y$ or model hyperparameters $\theta$.

4.2 Basis Functions

The process function in Eq. (4.2) is a GP with an assumed zero mean; however, many processes that follow a distribution have non-zero mean. For some processes with non-zero means, it might be possible to provide an explicit function describing the mean response as a function of the independent variables $x$. In the case where an explicit $\mu(x)$ is not available, an alternative is to use model basis functions that can incorporate information about the process from another data source. Gaussian process regression readily facilitates incorporating model basis functions, i.e., calibrating one data set’s surrogate model using another data set in the model basis functions. Basis functions can improve the GP surrogate modeling, as Section 4.2.2 will demonstrate. Multiple authors show methods of using the response from one data source (e.g., low-fidelity data) as a model basis function to help the Gaussian process model represent the response from another data source (e.g., high-fidelity
data) [23, 34, 35, 38–40]. For the aerodynamic merging work, the ability to use model basis functions provides an advantage to building a surrogate of the wind tunnel $C_p$ distribution, because the observations from the wind tunnel are quite sparse in the $\eta$ dimension.

This paragraph describes two equivalent methods of writing the GP model expressions with the model basis function. Rasmussen and Williams [23] provide another version of the observed response equation in Eq. (4.1) but with an additional regression term as the mean function. Their equation for the process with model basis functions is

$$y(x) = g(x) + \epsilon = f(x) + H(x, y^m)\beta + \epsilon, \quad f(x) \sim \mathcal{N}(0, K).$$

They changed the process notation from $f(x)$ in Eq. (4.1) to $g(x)$ here so that the marginal likelihood and predictive equations for $f(x)$ in Eqs. (4.8), (4.12), and (4.13) would not be confused with the marginal likelihood and predictive equations for the process, $g(x)$, that include the model basis function. So, the zero-mean assumption for $f(x)$ remains unchanged. $H$ is a basis regression function matrix with scale and location corrections of the model basis function $y^m$ and $\beta$ are the regression parameters. Kennedy and O’Hagan [34, 38] and Vanli et al. [40] write the expression in Eq. (4.14) using different nomenclature

$$y(x) = g(x) + \epsilon = \delta(x) + \rho(x)y^m(x) + \epsilon$$

where $\delta$ and $\rho$ are the location and scale correction functions, respectively, to the model basis $y^m$. The processes, $g(x)$, in Eqs. (4.15) and (4.14) are equivalent. To prove this assertion, consider correction terms and basis functions in the respective equations. Correction terms on the right hand side of Eq. (4.15) using first-order polynomials in the $d$-dimensional independent variable vector $x$ for both location and scale correction functions are (see Refs. [34, 40])

$$\delta(x) = [1, x_1, \cdots, x_d] [\delta_0, \delta_1, \cdots, \delta_d]^\top + W_\delta(x), \quad W_\delta(x) \sim \mathcal{N}(0, K)$$

$$\rho(x)y^m = [1, x_1, \cdots, x_d] [\rho_0, \rho_1, \cdots, \rho_d]^\top y^m.$$
Rewriting Eq. (4.15) with the terms in Eqs. (4.16) and (4.17) becomes

\[
\mathbf{y}(\mathbf{x}) = [1, x_1, \cdots, x_d] [\delta_0, \delta_1, \cdots, \delta_d]^\top + W_\delta(\mathbf{x}) + [1, x_1, \cdots, x_d] [\rho_0, \rho_1, \cdots, \rho_d]^\top \mathbf{y}_m + \epsilon. \tag{4.18}
\]

Thus, \(f(\mathbf{x})\) and \(W_\delta(\mathbf{x})\) from Eqs. (4.14) and (4.16), respectively, are identical (once again, assuming that \(f(\mathbf{x})\) in Eq. (4.2) has a zero mean). The basis functions and regression parameters from Eq. (4.14), with linear \(x\) terms, are

\[
H(\mathbf{x}, \mathbf{y}_m)\beta = \begin{bmatrix}
1 & x_{1,1} & \cdots & x_{1,d} & y^m(\mathbf{x}_1) & y^m(\mathbf{x}_1)x_{1,1} & \cdots & y^m(\mathbf{x}_1)x_{1,d} \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
1 & x_{N,1} & \cdots & x_{N,d} & y^m(\mathbf{x}_N) & y^m(\mathbf{x}_N)x_{N,1} & \cdots & y^m(\mathbf{x}_N)x_{N,d}
\end{bmatrix} \beta
\]

\[
\beta = [\delta_0, \delta_1, \ldots, \delta_d, \rho_0, \rho_1, \ldots, \rho_d]^\top. \tag{4.19}
\]

The regression parameter value estimates are calculated with Eq. (4.25) after estimating the GP model hyperparameters. The basis regression matrix \(H\) in Eq. (4.19) is valid for an arbitrary number of \(d\) variable dimensions; this aerodynamic data merging used \(d = 2\) for \(s\) and \(\eta\). Therefore, \(g(\mathbf{x})\) from Eqs. (4.15) and (4.14) are equal

\[
\delta(\mathbf{x}) + \rho(\mathbf{x})y^m(\mathbf{x}) = g(\mathbf{x}) = f(\mathbf{x}) + H(\mathbf{x}, y^m)\beta. \tag{4.20}
\]

Figure 4.1 shows the impact of including a model basis function in the GP regression model to represent the wind tunnel \(C_p\) distribution. In both plots of Fig. 4.1, the \(C_p\) measurement values from the wind tunnel appear as points, the mean of the GP prediction of \(C_p\) appears as a solid red line, and the mean of the GP prediction plus or minus the variance of the GP prediction appears as dotted red lines above and below the solid red line. The plot in Fig. 4.1a shows the GP prediction of the wind tunnel \(C_p\) data without a model basis function; here the mean prediction passes through all of the observed data points, but the uncertainty associated with the predictor is very high for values of \(s\) far from the pressure port locations. Figure 4.1b shows the GP prediction when the B-spline surrogate of the \(C_p\) values serves as the model basis function. With this model basis function, the mean GP prediction no longer passes
Figure 4.1.: Impact of the model basis function from Eq. (4.15) or (4.14) on the GP prediction of $C_p$ on the slat element at $\eta = 0.98$, $\alpha = 13^\circ$.

exactly through the observed wind tunnel $C_p$ values, but the associated prediction uncertainty is greatly reduced. The model basis function provides a baseline off of which the GP regression model can build; the model function provides structure to the calibrated data surrogate. This is especially evident where the calibrated data surrogate, here WT $C_p$ values, has few or missing data across a range of the independent variable(s). For the Trap wing model, the region $0 < s < 0.4$ corresponds to the lower surface of the slat trailing edge to nearly the slat leading edge; no pressure measurements were received from this portion of the slat.

The construction of GP predictions of the wind tunnel $C_p$ distribution as a function of arc length at the span locations corresponding to pressure port bands on all three elements of the Trap Wing demonstrated that the WT GP model, when using the B-spline surrogate of the CFD results at the same spanwise locations as the model basis functions, generally follows the shape of the CFD model basis function where no WT data points exist. Additionally, the GP model’s slope far from the measured WT data points seems to closely approximate the GP model’s slope at the closest WT data points; this is notably different from the behavior of the GP prediction that
does not use the CFD B-spline as a model basis function. Figure 4.1a illustrates the mean prediction for response values far from data points when the GP model uses no model basis function. This linear trend is due to the linear scale and location correction functions in Eq. (4.19). The positive or negative slope of the GP mean prediction when no model basis function exists, and in regions with no WT data (e.g.; $s \in [0, 0.4]$ in Fig. 4.1a), depended on the positive, or negative, sign of the estimated hyperparameter values. In Fig. 4.1a, with $s$ as the only independent variable, the term $d_1$ must have a positive value, so that the mean $C_p$ prediction looks to be a linear function of $s$ with positive slope for $s \in [0, 0.4]$. Similarly, constructing GP predictors of the same data in Fig. 4.1a with constant or quadratic polynomial correction terms and no model basis functions generated mean functions with constant and quadratic predictions in regions without WT data.

The regression parameters, $\beta = \{\delta, \rho\}^\top$, can have a variety of imposed priors (i.e., an assumption about the probability distribution for the response), but the distribution of the priors will determine which method (Bayesian inference or MLE) is best to estimate the hyperparameters $\theta$. For example, specifying any type of distribution function for the priors on the regression parameters requires estimating the GP model hyperparameters, $\theta$ (signal variance and length scale parameters for the process covariance functions $K$ and Gaussian noise $\epsilon$, but not regression parameters $\beta$), via Bayesian inference sampling. However, both Bayesian inference sampling and maximum likelihood estimation (or log marginal likelihood) can generate GP hyperparameter estimates for normally distributed or vague priors on $\beta$ (see Section 2.7 of Ref. [23] for more details). The log marginal likelihood from Ref. [23] for $y(x) = g(x) + \epsilon$ with vague $\beta$ priors is

$$\log p(y|x) = -\frac{1}{2} \left[y^\top M^{-1} y - y^\top C y + \log |M| + \log |A| + (n - m) \log 2\pi \right] \quad (4.21)$$

where $M = K + \sigma^2 I$, $A = H M^{-1} H^\top$, $C = M^{-1} H^\top A^{-1} H M^{-1}$, $n$ is the number of data points, and $m$ is the rank of $H^\top$, which depends upon the basis functions used for location and scale correction. The log marginal likelihood in Eq. (4.21) does
not have any reference to the regression parameters $\beta$ because of the assumed vague priors.

Once the likelihood maximization determines the hyperparameters, then the mean and covariance predictive equations for Eq. (4.14) with vague $\beta$ priors are

$$g(x_*) = \bar{f}(x_*) + \mathbf{R}^T\bar{\beta}$$

$$= \mathbf{K}^*_s\mathbf{M}^{-1}\mathbf{y} + \mathbf{R}^T\bar{\beta}$$

$$\text{cov}(g_*) = \text{cov}(f_*) + \mathbf{R}^T(\mathbf{H}^{-1}\mathbf{H}^T)^{-1}\mathbf{R}$$

$$= \mathbf{K}^*_s - \mathbf{K}^*_s\mathbf{M}^{-1}\mathbf{K}^*_s + \mathbf{R}^T(\mathbf{H}^{-1}\mathbf{H}^T)^{-1}\mathbf{R}$$

where

$$\mathbf{R} = \mathbf{H}^*_s - \mathbf{H}^{-1}\mathbf{K}^*_s, \quad (4.24)$$

$$\bar{\beta} = (\mathbf{H}^{-1}\mathbf{H}^T)^{-1}\mathbf{H}^{-1}\mathbf{y}, \quad (4.25)$$

$\mathbf{H}_s$ are basis functions from Eq. (4.19) at test points $x_*$, and $\bar{f}(x_*)$ and $\text{cov}(f_*)$ come from Eqs. (4.12) and (4.13), respectively. In the aerodynamic data merging application, the mean prediction in Eq. (4.22) would be the prediction of the WT $C_p$ values at locations $x_*$ on the wing.

See Ref. [23] for the log marginal likelihood, mean predictive, and covariance predictive equations if normal priors are chosen for $\beta$. Imposing vague priors on $\beta$ is most relevant for the WT $C_p$ surrogate model because the user is not likely to have a good grasp on the value and distribution of the regression parameters $a\ priori$ to building the GP surrogate.

### 4.2.1 Correction Functions

The location and scale correction basis functions in Eq. (4.19) do not necessarily need to be linear when using a model response function $y^m(x)$ in the GP model to provide a surrogate of measured data. Authors conducting research in areas not related to modeling $C_p$ indicated a preference for constant correction polynomial terms.
(Refs. [33, 34, 39, 41–43]), a couple authors used a linear set of correction functions (Refs. [34, 40, 44]), Reese et al. [35] explore model results using scale correction terms with linear and cross product terms, and Ling, Mullins, and Mahadevan [45] develop various location correction function formulations.

The author investigated the impact of constant, linear, and quadratic scale and location correction functions for the aerodynamic data merging. The linear correction functions are already provided in Eq. (4.19); the constant and quadratic basis functions are provided below. The constant correction functions are

\[
\delta(x) = \delta_0 + W_\delta(x) \tag{4.26}
\]

\[
\rho(x)y^m = \rho_0 y^m \tag{4.27}
\]

or

\[
H(x)\beta = \begin{bmatrix}
1 & y^m(x_1) \\
\vdots & \vdots \\
1 & y^m(x_N)
\end{bmatrix} \beta
\]

\[
\beta = [\delta_0, \rho_0]^T. \tag{4.28}
\]

This work did not consider interaction terms in the quadratic correction functions

\[
\delta(x) = [1, x_1, \cdots, x_d, x_1^2, \cdots, x_d^2] [\delta_0, \delta_1, \cdots, \delta_d, \delta_{d+1}, \cdots, \delta_{2d}]^T + W_\delta(x) \tag{4.29}
\]

\[
\rho(x)y^m = [1, x_1, \cdots, x_d, x_1^2 \cdots, x_d^2] [\rho_0, \rho_1, \cdots, \rho_d, \rho_{d+1}, \cdots, \rho_{2d}]^T y^m. \tag{4.30}
\]

Similar adaptations can be made for other polynomial, or non-polynomial basis functions. As Section 4.2.2 will discuss, the author found through experimentation with the WT $C_p$ distributions that linear correction terms provided a good compromise of approximating the data and lower computational cost than those associated with quadratic correction functions (see Section 4.2.2).

Another option is not including the model response, $y^m$, in the basis functions. This would result in only $\delta$ regression parameters. This may be required where there is no other data source and the user wants to incorporate possible offset, or location,
corrections through the $\delta$ functions. For this aerodynamic data merging application, the fact that the B-spline representing the CFD generated $C_p$ distribution is available to provide information about the $C_p$ distribution in the wing span locations between pressure tap rows means that using $y^m$ seems to be a more appropriate approach.

4.2.2 Comparing Polynomial Correction Functions

This section demonstrates and discusses examples of constant, linear, and quadratic polynomial location and scale correction functions in the effort to provide an appropriate representation of the wind tunnel $C_p$ distribution, given that the B-spline surrogate for the CFD $C_p$ distribution is available as a model function.

Figure 4.2 shows the GP regression model results for constant, linear, and quadratic correction functions. The models provide approximations to NASA Trap Wing wind tunnel (WT) data on the flap wing element at the wing tip, $\eta = 0.98$ pressure tap row, for $\alpha = 21^\circ$. Comparisons at other spanwise locations and other wing elements consistently produced similar results. Several options exist for the covariance function $K$ when building a GP model (Eq. (4.9) showed the squared exponential form). For the comparisons made in Fig. 4.2, $K$ employs a summation of neural network (NN) and rational quadratic (RQ) terms. This combination appears to work best for this application; Section 4.3, ahead in the document, will discuss covariance functions and an investigation of these for this application. The model basis function $y^m$ is the CFD cubic B-spline surrogate approximation. The noise is modeled as a zero mean Gaussian distribution with constant variance, $\epsilon \sim \mathcal{N}(0, \sigma^2)$. In Fig. 4.2, the GP mean prediction of the WT $C_p$ appears as the solid red line; the GP covariance prediction gives an idea of the uncertainty in the prediction and appears as the dotted red line above and below the mean prediction. The $C_p$ values at each pressure tap based upon the wind tunnel data appear as green symbols. Values from the B-spline surrogate for the CFD $C_p$ values appear as the small blue symbols.
The linear correction functions appear to produce slightly better approximations than the constant correction functions near the flap leading edge and upper surface ($s > 0.5$) because it captures the pressure rise more accurately. However, the opposite is true on the lower surface, especially near $s = 0.2$ where the GP mean prediction with the linear corrections results in $C_p$ values much smaller in magnitude than was actually measured; the constant corrections approach provides a better match near the lower surface trailing edge. The quadratic correction function seems to approximate the WT data very well at the data points, but seems to over-fit the data near the lower surface.
Table 4.1: Correction function computational cost and error comparison for the flap WT GP model at $\eta = 0.98$, $\alpha = 21^\circ$

<table>
<thead>
<tr>
<th>Polynomial correction</th>
<th>Time (sec)</th>
<th>RMSE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Constant</td>
<td>40.7</td>
<td>0.206</td>
</tr>
<tr>
<td>Linear</td>
<td>43.8</td>
<td>0.185</td>
</tr>
<tr>
<td>Quadratic</td>
<td>44.5</td>
<td>0.026</td>
</tr>
</tbody>
</table>

surface trailing edge ($s \approx 0$) where the GP mean prediction has additional curvature between the pressure taps on this part of the flap. Perhaps even more evidence of the over-fitting is the rapid decrease in predicted $C_p$ magnitude between the aft most pressure tap and the flap trailing edge. As the model basis function, $y^m$, the CFD B-splines predictions “guide” the shape of the WT GP model distribution away from the measured data points, but the GP surrogate approximates the WT $C_p$ values as much as possible despite the fact that the CFD B-spline surrogate $C_p$ predictions are much lower than the WT data. The difference between the CFD and WT $C_p$ data was a common occurrence at the First AIAA CFD High-Lift Prediction Workshop [3].

Table 4.1 enumerates the computational cost and surrogate modeling approximation error in Fig. 4.2. The computational cost is characterized by the time to execute the MATLAB script on a Dell Optiplex 7010 with a third generation core i7 processor and 8 GB of RAM. The root-mean-square error (RMSE) is

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (y(x_i) - \hat{y}(x_i))^2}. \quad (4.31)$$

In this example, the data is $y(x_i) = C_{p,WT}(s_i)$ and the approximation is $\hat{y}(x_i) = \hat{C}_{p,WT}(s_i)$. The computational cost between different surrogates is comparable, but slightly increases with increasing polynomial degrees, and thus, with increasing degrees of freedom. The RMSE values decrease with increasing degrees of freedom. The computational cost and error trends hold for other wing elements and other spanwise locations. In spite of the much lower RMSE values when using quadratic correction
functions, the concern about over-fitting and slight increase in computational cost lead the author to select the linear location and scale correction functions for constructing the WT surrogate model, with the B-spline surrogate of the CFD results as $y^m(x)$.

### 4.3 Covariance Functions

Covariance function characteristics greatly influence Gaussian process model performance as surrogate models. A covariance function is a mapping indicating the relationship between two inputs. The covariance function for a real-valued function, from Section 4.1, is

$$K(x, x') = \text{cov}(f(x), f(x'))$$

$$= \mathbb{E} [(f(x) - \mu(x))(f(x') - \mu(x'))^\top]. \quad (4.32)$$

The covariance function assumes that different vectors of independent variables, for instance, $x$ and $x'$ in Eq. (4.32), that are close in value(s) have output responses that are closely correlated. The level and behavior of that correlation depends on how close the input values are to each other (i.e., the distance between $x$ and $x'$), the kernel or covariance function form chosen by the user building the GP model, and the kernel parameter values that are determined either through maximizing the log-likelihood or Bayesian inference.

Several options for kernel functions exist for GP models; this research considered the four options listed in Table 4.2 and others (e.g., gamma-exponential) discussed in Ref. [23], but the four in Table 4.2 proved to provide consistently greater flexibility in representing WT $C_p$ data. Data characteristics (e.g., general trends, periodicity, noise, and irregularities or departures from the model basis function) drive the choice of kernel functions (see Ref. [23]). Among all considered kernels for this research, the neural network provided the greatest capability in representing the $C_p$ distributions for all wing elements (this is evident in main effects plots in Section 4.3.2). In the squared exponential, rational quadratic, and Matérn equations, the scalar distance
Table 4.2: Kernel expressions

<table>
<thead>
<tr>
<th>Covariance function</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Squared Exponential</td>
<td>$k_{SE}(r) = \sigma_{SE}^2 \exp\left(-\frac{r^2}{2l^2}\right)$</td>
</tr>
<tr>
<td>Rational Quadratic</td>
<td>$k_{RQ}(r) = \sigma_{RQ}^2 \left(1 + \frac{r^2}{2\gamma^2}\right)^{-\gamma}$</td>
</tr>
<tr>
<td>Neural Network</td>
<td>$k_{NN}(\mathbf{x}, \mathbf{x}') = \sigma_{NN}^2 \frac{2\sin\left(\frac{2\Sigma \Sigma'}{\sqrt{(1+2\Sigma \Sigma') (1+2\Sigma' \Sigma')}}\right)}{\pi}$</td>
</tr>
<tr>
<td>Matérn</td>
<td>$k_{Mat}(r) = \sigma_{Mat}^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{2\nu r}{l}\right)^{\nu} K_{\nu}\left(\frac{\sqrt{2\nu r}}{l}\right)$</td>
</tr>
</tbody>
</table>

between two points $r = |\mathbf{x} - \mathbf{x}'|$. In the neural network equation, the column vector describing a combination of independent variables $\mathbf{x} = (1, x_1, \ldots, x_d)^\top$ (Ref. [23] uses this simple concatenation of the constant one and the $\mathbf{x}$ vector for a single data point location.). Finally, in the Matérn function, $K_{\nu}$ is a modified Bessel function and $\Gamma$ is the gamma function. The parameters for each kernel include the signal variances, $\sigma^2$, and various length scales. The length scales for the corresponding kernels are: $l$ for the squared exponential (SE), $\gamma$ and $l$ for the rational quadratic (RQ), $\Sigma = \text{diag}(\sigma_0, \sigma)$ for the neural network (NN), and $\nu$ and $l$ for the Matérn. When constructing the GP model, these length scales are part of the hyperparameters that are determined via the log-likelihood maximization. The diagonal matrix of $\sigma_0$ and $\sigma$ (both unknowns) for the NN kernel define the offset from the origin and x-axis scaling, respectively.

The Matérn kernel expression turns into a much simpler expression that is the product of an exponential function and a polynomial when $\nu$ is a half-integer value: $\nu = h + 1/2$

$$k_{\nu=h+1/2}(r) = \sigma_{Mat}^2 \exp\left(-\frac{\sqrt{2\nu r}}{l}\right) \frac{\Gamma(h+1)}{\Gamma(2h+1)} \sum_{i=0}^{h} \frac{(h+i)!}{i! (h-i)!} \left(\frac{\sqrt{8\nu r}}{l}\right)^{h-i}.$$ (4.33)

Rasmussen and Williams [23] demonstrate that the GP for $\nu = 1/2$ is not smooth (very rough), and that distinguishing between kernels with $\nu \geq 7/2$ is difficult. So,
using values of \( \nu = 3/2 \) and \( 5/2 \) is more practical when considering the Matérn kernel function as an option for a GP model. These functions are

\[
k_{\nu=3/2}(r) = \sigma_{\text{Mat}}^2 \exp \left( -\frac{\sqrt{3}r}{l} \right) \left( 1 + \frac{\sqrt{3}r}{l} \right)
\]

\[
k_{\nu=5/2}(r) = \sigma_{\text{Mat}}^2 \exp \left( -\frac{\sqrt{5}r}{l} \right) \left( 1 + \frac{\sqrt{5}r}{l} + \frac{5r^2}{3l^2} \right)
\]

(4.34)

(4.35)

This simplification greatly reduces the computational expense because the kernel no longer needs to calculate the modified Bessel and Gamma function values.

The squared exponential kernel is probably the most common among all of the kernels [23]. This kernel is very similar to the kriging surrogate model covariance function; in recent years, kriging models have received increasing popularity as surrogate models in a variety of applications including for design optimization. The kriging surrogate model is a subset of the Gaussian process model. To extract the kriging surrogate from the GP model, simplify Eq. (4.15) by removing the model basis function / scale correction term, the noise term \( (\epsilon) \), and assume a constant correction function. The kriging covariance function is

\[
k(x, x') = \sigma^2 \exp \left( -\sum_{i=1}^{d} \theta_i \left| \frac{x_i - x_i'}{2} \right|^{p_i} \right)
\]

(4.36)

where \( \theta_i \) are the length scale parameters for \( d \) variable dimensions and \( p_i \) are a smoothness parameters on the interval \( 0 < p_i \leq 2 \). The smoothness parameters are often (Refs. [7, 33, 46–48]) set to \( p_i = 2 \) to “[give] a process with infinitely differentiable paths” [33]; with \( p_i = 2 \), the kriging kernel is the squared exponential kernel in each variable dimension \( d \). Because this most common form of the kriging model is the squared exponential kernel, there is no need to investigate it separately from the four selected forms.

4.3.1 Combining Kernels to Create New Kernels

In addition to using a single kernel function when constructing a GP model, kernels can be combined in multiple ways to create new kernels. The following discussion
is derived from Ref. [23] and is useful to describe the kernels in this work, because investigations revealed that combinations of kernels were necessary to best represent the wind tunnel $C_p$ distribution via a GP model.

The addition of two kernels is also a kernel. Suppose a random process is the sum of two independent random processes, $f(x) = f_1(x) + f_2(x)$. Then, the kernel $k(x, x') = k_1(x, x') + k_2(x, x')$. This addition property allows combining various kernels with different characteristics and length scales to increase the flexibility (by adding degrees of freedom of the model) and improve the surrogate modeling. For example, combining two SE kernels can allow the GP model to account for two different trends in the data, e.g., long and short-term trends.

The product of two kernels is also a kernel. Once again, suppose a random process that is the product of two independent random processes, $f(x) = f_1(x)f_2(x)$. Then, the kernel $k(x, x') = k_1(x, x')k_2(x, x')$ is also a valid kernel. Combining the above addition and multiplication methods would also result in a valid kernel, $k(x, x') = k_1(x, x') + k_2(x, x') + k_3(x, x')k_4(x, x')$, if the random process to be modeled was a combination of other independent random processes, $f(x) = f_1(x) + f_2(x) + f_3(x)f_4(x)$.

Additionally, suppose a random process $f(x)$ is a function of $d$-dimensional variables $x$. For those dimensions that are independent from each other, the additive function model is $f(x) = C + \sum_{i=1}^{d} f_i(x_i)$. The resulting covariance function is an additive combination of kernels for each dimension. When $x$ dimensions interact, the function has additional interaction terms, so that $f(x) = C + \sum_{i=1}^{d} f_i(x_i) + \sum_{i=2}^{d} \sum_{j=1}^{i-1} f_{ij}(x_i, x_j)$. The resulting covariance function for a GP model of this process is

$$k(x, x') = \sum_{i=1}^{d} k_i(x_i, x'_i) + \sum_{i=2}^{d} \sum_{j=1}^{i-1} k_{ij}(x_i, x_j; x'_i, x'_j).$$

(4.37)

Wahba [49] suggests using tensor products so that $k_{ij}(x_i, x_j; x'_i, x'_j)$ interacting kernels becomes $k_{ij}(x_i, x'_i)k_{ij}(x_j, x'_j)$. In the two-dimensional space the kernel is $k(x, x') = k_1(x, x') + k_2(x, x') + k_3(x, x')k_4(x, x')$. Note that through the simple commutative property $k_2(x, x')k_1(x, x') = k_1(x, x')k_2(x, x')$. 
4.3.2 Comparing Kernels

With a variety of kernel functions available, and with the ability to combine kernel functions via addition and multiplication, the best kernel function to use in a GP surrogate model of the $C_p$ distribution is not obvious. This section discusses a study to investigate the various kernel options. The Gaussian process (GP) equations in the preceding sections allow for surrogate models in an arbitrary number of dimensions. While previous examples only examined data in the arc length dimension, this section discusses a sensitivity study of how GP covariance kernels in arc length and span affect two-dimensional (2-D) wind tunnel (WT) GP surrogate models. A Design of Experiments (DOE) approach provides the various combinations of kernel functions to employ for each experiment run (i.e., the sampling pattern) using a full factorial design. Each experiment run, or “trial,” uses a specific combination of kernel functions specified by the full factorial DOE. The GP covariance kernels are the study factors, or variables, and the mean absolute error (MAE) of the 2-D GP surrogate is the study response metric for each wing element and angle of attack. Thus, lower MAE values indicate that the surrogate is a better approximation of the data. Main and interaction effect plots indicate the sensitivity of the surrogate model to specific kernels.

A two-level full factorial experiment determines the factor level sampling pattern. There are seven factors in this Design of Experiments study corresponding to the covariance kernel choices; four from arc length and three from span directions. The four arc length direction factors correspond to the considered kernel functions in Table 4.2; these are neural network (NN), rational quadratic (RQ), squared exponential (SE), and Matérn (Mat) kernels. The three span direction factors are neural network (yNN), squared exponential (ySE), and Matérn (yMat) kernels, where the ‘y’ prefix sets it apart as a span kernel. The rational quadratic kernel is not employed as a factor in the spanwise direction because experience indicated it was not as important in this direction, and to decrease the study computational cost. The DOE employs
a two-level design (±1), which indicate whether or not the GP model utilizes the factor (i.e., kernel) in each trial. A full factorial experiment design with seven factors at two levels each requires \( N = 2^7 \) (128) experiments. The high and low (+1 and −1, respectively) level settings indicate the kernel is and is not used, respectively. The kernels in the same dimension were added, and kernels between dimensions were combined using Eq. (4.37) with both additive and multiplicative terms because there is a possibility for the air flowing over the wing to have cross flow in the spanwise direction producing an interaction effect between arc length and spanwise pressure values. For example, if the arc length direction had NN and SE kernels and the spanwise direction had the yMat kernel, then the resulting kernel \( k \) would be

\[
k_s(x, x') = k_{NN}(x, x') + k_{SE}(x, x')
\]

\[
k(x, x') = k_s(x, x') + k_{yMat}(x, x') + k_s(x, x')k_{yMat}(x, x')
\]

where \( k_s \) is the combined arc length kernel. The kernel equations are represented in Table 4.2, and the Matérn kernel uses the \( \nu = 5/2 \) simplification from Eq. (4.35) because of the recommendation in Ref. [23] and for computational convenience. The author’s experience indicated that either \( \nu = 3/2 \) or \( \nu = 5/2 \) provided similar results, but \( \nu = 5/2 \) has more flexibility because of the additional term in the kernel expression. The hyperparameters for each DOE experiment included the signal amplitudes (variances) and length scales for the combined kernel, as in Eq. (4.39), and the single noise variance term, \( \sigma^2 \), as in Eqs. (4.1) and (4.15).

Factorial experiments in DOE use replicates to account for experimental error and decrease the sample mean variance (see Section 1-3 of Ref. [15]). Replicates are repeated experiment runs at the same factor levels. This work used a single replicate, \( n = 1 \), or an “unreplicated factorial” because the maximum log marginal likelihood estimate results were sufficiently consistent, i.e., nearly deterministic, as to not warrant additional computational expense in calculating replicates (The differential evolution algorithm that calculates the hyperparameters is stochastic in nature, but the consistency of the results indicated near-deterministic behavior.) [15]. The
order of experiment runs should generally be randomized to eliminate any impact that the run order of experiments may have on the response(s). However, the order of computer experiments does not impact the results, so experiment run order randomization was not implemented here.

Equations (6-22) and (6-23) in Ref. [15] are the effect estimate and sum of squares equations for full factorial designs. The $i^{th}$ effect estimate from Eq. (6-22) is

$$i = \frac{2}{n2^k} (\text{Contrast}_i)$$

where $N = n2^k$. In this work, $n = 1$, $k = 7$ and $N = 128$. The general equation for a contrast of effect $AB \cdots K$ is

$$\text{Contrast}_{AB\cdots K} = (a \pm 1)(b \pm 1) \cdots (k \pm 1)$$

where $a, b, \cdots k$ represent factorial experiments with the $A, B, \cdots K$ factors at the high levels. Note that the negative in the parenthesis is if the factor is included in the contrast, and the positive is for when the factor is not included. The following example comes from Ref. [15]. An example factorial experiment has three factors ($A$, $B$, and $C$) at two levels ($2^3$). The contrast for the $AB$ two-factor interaction is

$$\text{Contrast}_{AB} = (a - 1)(b - 1)(c + 1)$$

$$= abc + ab + c + (1) - ac - bc - a - b,$$

while the contrast for the main effect $A$ is

$$\text{Contrast}_A = (a - 1)(b + 1)(c + 1)$$

$$= abc + ab + ac + a - bc - b - c - (1).$$

For details on calculating effect estimates for fractional factorial designs, see section (8-4.2) of Ref. [15].

The slat, spar, and flap wing elements have 102, 240, and 168 port locations, respectively. So, the MAE summary metric for each wing element combines the 2-D GP surrogate error (residuals) across all pressure ports into one response metric.
Table 4.3: Kernel factors and levels

<table>
<thead>
<tr>
<th>Factor</th>
<th>Name</th>
<th>Low Level</th>
<th>High Level</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Neural Network (NN)</td>
<td>off</td>
<td>on</td>
</tr>
<tr>
<td>B</td>
<td>Rational Quadratic (RQ)</td>
<td>off</td>
<td>on</td>
</tr>
<tr>
<td>C</td>
<td>Squared Exponential (SE)</td>
<td>off</td>
<td>on</td>
</tr>
<tr>
<td>D</td>
<td>Matern $\nu = 5/2$ (Mat)</td>
<td>off</td>
<td>on</td>
</tr>
<tr>
<td>E</td>
<td>Neural Network (yNN)</td>
<td>off</td>
<td>on</td>
</tr>
<tr>
<td>F</td>
<td>Squared Exponential (ySE)</td>
<td>off</td>
<td>on</td>
</tr>
<tr>
<td>G</td>
<td>Matern $\nu = 5/2$ (yMat)</td>
<td>off</td>
<td>on</td>
</tr>
</tbody>
</table>

The mean absolute error (MAE) transforms negative residual values into the positive range, and then calculates an average.

Figure 4.3 contains the MAE main effects for the slat at $\alpha = 6^\circ$. The y-axis contains the mean of the MAE metric, and the 0 and 1 values on the x-axis indicate that the kernel is not and is used, respectively. The larger the slope of the line for each main effect, the greater the effect that factor has on the response. Thus, visual inspection indicates that the order of factor importance for the slat at $\alpha = 6^\circ$ is A, C, D, B, E, F, and finally G. It is interesting that the arc length factors are all more important than the spanwise kernel factors in the MAE; this is likewise true for the $L^2$-norm and RMS metrics (see Appendix B). The main effects plot would induce the engineer to not use the ySE or yMat, and maybe not even the yNN or RQ kernels. Another set of plots that can help determine which factors are significant are normal probability plots of the effect estimates from Eq. (4.40) and interaction plots between the factors. The normal probability plot of the slat effect estimates in Fig. 4.4 illustrate which main effects and interaction effects are significant by which variables deviate from the red line. All main and interaction effect estimates ($A, B, \ldots, ABCDEFG$) are included in Fig. 4.4. The further the effect estimate from the red line, whether on the positive or negative side, the greater the effect significance.
Figure 4.3.: Slat 2-D WT GP MAE main effects for $\alpha = 6^\circ$.

Figure 4.4.: Normal probability plot for the slat 2-D WT GP MAE effect estimates for $\alpha = 6^\circ$. 
Thus, factor $A$ has the greatest impact on the slat MAE metric for $\alpha = 6^\circ$, which validates the conclusions from the main effects plot in Fig. 4.3. Also, the conclusions drawn on the order of factor importance from Fig. 4.3 is also validated in Fig. 4.4. The interaction effects of $AC$, $AD$, and $ABCD$ all have greater impact on the MAE metric than the $E$ main effect. From this plot, the engineer would probably choose to use the NN, RQ, SE, and Mat kernels in the arc length direction no specific kernel in the span direction, while also including the constant noise kernel. Since the normal probability plot indicated that interaction effects are significant, it is important to generate an interaction effects plot for examination.

Figure 4.5 is a two-factor interaction effects plot. The interaction effects plot

![Two-factor interaction effects plot](image)

Figure 4.5.: Slat 2-D WT GP MAE two-factor interaction effects for $\alpha = 6^\circ$ blue and dotted lines are for the row variable not turned on and turned on, respectively.

has the main factors on the diagonal and the interactions between those two factors on the off-diagonal plots. The 0 and 1 for each plot are the low and high levels, respectively, for the factor in that column—the left-most column of plots have the low level of factor $A$ on the left and the high level on the right. The blue solid
and dotted lines indicate the low and high factor levels, respectively, for the factor in that row—the top row of plots has the low level of factor A as the blue line and the high level as the dotted line. Two-factor interaction plots obviously do not account for higher-level interactions, e.g., $ABCD$, but these interactions are not as significant has two-factor interactions, as illustrated in Fig. 4.4. The large number of interaction plots in Fig. 4.5 provide a rich set to explain how interaction plots can be interpreted, as well as validating the significant kernel factor interactions for the slat 2-D GP at $\alpha = 6^\circ$ from Fig. 4.4. Parallel solid and dotted lines indicate that there is no interaction between the main factors, e.g., the plots for the $BC$ two-factor interaction. There are multiple examples here of no two-factor interactions, e.g., $BD, CE, DE, BG$, and so on. Horizontal lines indicate that there is no main effect, e.g., the plots for the $FG$ two-factor interaction. These plots also show no interaction. Plots with solid and dotted lines close together mean that the main factor in that row does not impact the MAE error metric very much, e.g., rows for factors $E, F,$ and $G$. On the other hand, rows with lines farther apart mean the main effect in that row is more significant, e.g., the top row for factor $A$. Interaction plots where the lines have different slopes, e.g., the factor $A$ column with the rows for factors $B, C,$ and $D$, show that one factor has a larger impact on the results than the other, and that there is a two-factor interaction effect. For example, in the $A$ factor column on the left (NN kernel) the MAE error does not change as much for high level $A$ (NN kernel used in GP model) regardless of the other factors’ levels. However, when the $A$ factor is not used (low level, or 0 on the plot) changing the other factors’ levels (low to high levels, or solid to dotted lines) creates a much larger change in MAE values than when $A$ is at the high level. Also, the plots for the $AC$ interaction shows a stronger interaction than for any other interaction based on the larger difference in the slopes of the solid and dotted lines; this interaction conclusion for factor $AC$ is validated by the normal probability plot in Fig. 4.4. Figure 4.5 definitely shows interaction among some of the factors, but the interactions are not as strong as if the solid and dotted lines crossed or had opposing slopes.
Figure 4.6 plots the main effects for the MAE error metric of the spar 2-D WT GP at $\alpha = 37^\circ$, and shows that the $A$ and $C$ factors are important, while the other factors may not be. Factors $E$, $F$, and $G$ do not appear significant in any way, but factors $B$ and $C$ may be; once again the normal probability of the effects and the two-factor interaction plots should be examined to determine which factors impact the GP surrogate’s ability to predict the WT $C_p$ data. The normal probability plot of the effect estimates for the spar in Fig. 4.7 illustrate and label the main effects and interaction effects that are significant. The $B$ and $D$ effect estimates and interaction effect estimates associated with these main effects are closer to the normal probability line indicating that they may not be significant. Figure 4.8 contains the two-factor interactions for the spar 2-D WT GP surrogate at $\alpha = 37^\circ$. One item of particular interest, from a training standpoint, in Fig. 4.8 is the $BE$ interaction. The interaction plot in row $B$ and column $E$ shows a positive and negative slope difference between the solid and dotted lines—this is called a crossover interaction. A crossover interaction is a stronger interaction than if the slope of the two lines were both positive or
both negative. The other interaction plot in row E and column B shows a crossover interaction where the lines cross, but have the same negative sign on the slope. If either B or E were significant main factors, a crossover interaction of these two factors would indicate a strong interaction that should be accounted for when building the GP surrogate. However, since neither of these factors is significant, the engineer would not be advised to use the corresponding kernels in the 2-D WT GP surrogate for this data.

Effects plots for the slat, spar, and flap at most angles of attack indicate that factor A (NN kernel) is consistently the most significant factor in lowering the MAE metric. The other arc length factors are also significant, and the effects plots show that the usual order of factor impact after A is C, D, and then B, corresponding to the SE, Mat, and RQ kernels. The author expected at least one spanwise kernel to be more significant than the effects plots indicate. Effects plots for other angles of attack and wing elements are provided in Appendix B.
Practically speaking, it is unlikely that the engineer would have the time or resources to conduct a statistical study to calculate statistically significant kernels to model and generate the aerodynamic database from the most recent set of CFD and WT experiments for an aircraft that needs to be designed immediately. However, the engineer may use Design of Experiments with aerodynamic data from a previous set of CFD and experimental data for a past aircraft design to determine the best kind of covariance functions to describe pressure distributions. This knowledge could help the engineer to understand which kernels perform best for the same type of data characteristics to expedite surrogate modeling efforts on current design problems.

The computational cost is another consideration to remember associated with using kernels. Increasing the number of kernels used in a single GP surrogate model, and hence, the degrees of freedom of the GP, increases the computational cost to generate the surrogates. Table 4.4 compares the total computational cost from the full factorial design study when the 2-D GP does not use any of kernels in arc length
and span and all kernels from Table 4.2 (not counting the constant variance noise kernel, $\sigma_n^2$, which is always used). This total cost sums the cost for GP models at all angles of attack ($\alpha = \{6, 13, 21, 28, 32, 34, 36, 37\}$). The total computational cost for the case when only using the noise kernel is on the order of a few minutes compared to multiple hours when employing all seven covariance kernels (NN, RQ, SE, Mat, yNN, ySE, and yMat) and the noise kernel. Thus, deciding on the smallest set of kernels to adequately represent the data could be beneficial to the engineer. Another response from each trial could be the time required to build the GP model (find the hyperparameters); then the user could consider this as a multi-objective problem to reduce error while also reducing computational cost. There may be a point of diminishing returns.

In conclusion, the author recommends using a statistical study to determine which covariance kernels to use in a specific application. There other methods to choose the appropriate model for a given application [23, 50]. For the aerodynamic data merging with the NASA Trap Wing WT data, the NN kernel in the arc length direction was nearly always the “best” kernel to use to decrease modeling error, but there were some angles of attack and wing elements where the SE kernel was more effective. There was no clear kernel choice in the spanwise direction.

<table>
<thead>
<tr>
<th></th>
<th>No Kernels</th>
<th>All Kernels</th>
</tr>
</thead>
<tbody>
<tr>
<td>Slat</td>
<td>3.98</td>
<td>381.5</td>
</tr>
<tr>
<td>Spar</td>
<td>4.49</td>
<td>248.7</td>
</tr>
<tr>
<td>Flap</td>
<td>2.17</td>
<td>162.5</td>
</tr>
</tbody>
</table>
4.4 Wind Tunnel Gaussian Process Surrogate Results

This section presents and discusses results of using GP surrogate models to represent the $C_p$ distribution of wind tunnel data on the NASA Trap Wing from the 1st AIAA CFD High Lift Prediction Workshop (HiLiftPW-1). The motivation is to provide the best possible representation of the $C_p$ distribution associated with the wind tunnel data—even (or perhaps especially) at locations on the wing not coincident with a pressure tap. As presented previously in Fig. 1.2, there are three different GP surrogate models shown here. The 1-D GP surrogates give an idea of how the approach building a surrogate of the wind tunnel data by using the B-spline for the CFD as a model basis function, but it cannot represent the $C_p$ over the entire surface of the wing. The other surrogates are the 2-D online GP surrogates (sequential GPs in arc length then span), and 2-D batch (an all-at-once model in arc length and span) GP surrogates.

Multiple authors used GP modeling for representing aerodynamic forces, e.g., lift or drag, [39, 51–54]. Leifsson and Koziel [55] and Koziel, Leifsson and Yang [56] employ a different surrogate modeling methodology, shape-preserving response prediction, to represent an airfoil’s pressure distribution to optimize the airfoil design. However, to date the author is unaware of work to construct surrogate models that represent the “field” of pressure distribution data in both arc length and span that is needed for aerodynamic data merging. This field of pressure data offers unique challenges in the modeling process, and addressing these challenges is a major portion of this research effort.

4.4.1 One-Dimensional Gaussian Process in Arc Length

The one-dimensional (1-D) Gaussian process (GP) surrogates in this section calibrate the WT $C_p$ surrogates in arc length with the model characteristics and setup in Table 4.5. The author selected the kernel combination based on the properties of each kernel described in Ref. [23], and extensive experience in modeling WT $C_p$
Table 4.5: 1-D GP model characteristics

<table>
<thead>
<tr>
<th>Characteristic</th>
<th>Value / Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model basis function</td>
<td>CFD B-spline</td>
</tr>
<tr>
<td>Scale &amp; location correction</td>
<td>linear (see Eq. (4.19))</td>
</tr>
<tr>
<td>Kernel</td>
<td>NN+SE+Mat</td>
</tr>
<tr>
<td>( \beta ) priors</td>
<td>vague</td>
</tr>
<tr>
<td>Measurement error</td>
<td>( \sigma^2 )</td>
</tr>
</tbody>
</table>

data from the Trap Wing. Following the discussion in Section 4.2, the B-spline surrogate of the CFD results provides the model basis function for these 1-D GP models. Maximizing the log marginal likelihood generated single-point estimates of the GP model hyperparameters, thus uncertainty bounds in plots for this section only reflect uncertainty in the mean prediction and cannot account for uncertainty in the WT data or model hyperparameters. The maximum likelihood estimation (MLE) method cannot incorporate data uncertainty into the calculation, even if the WT data had measurement uncertainty values (The NASA Trap Wing WT data provided mean and standard deviations on the wind tunnel flow conditions, e.g., Mach number and Reynolds number, but not on the pressure measurements [2].).

In Fig. 4.9, the GP surrogates at different spanwise locations (pressure port bands, or tap rows) and angles of attack show that the GP model works for many different conditions. These conditions may have 1) CFD and WT \( C_p \) data that are aligned, 2) clear differences in \( C_p \) values between the two data sources for some arc length locations, or 3) differences in \( C_p \) slope between CFD and WT data sources. The WT data and CFD B-spline \( C_p \) values at the port locations, \( C_{p,WT}(s_k) \) and \( \hat{C}_{p,CFD}(s_k) \), respectively, are closely aligned for the slat in Fig. 4.9a, so the one-dimensional surrogates are aligned as well. This agreement in WT data and CFD B-spline predictions is usually the case for all elements (slat, spar, and flap) at the inboard pressure port bands. The WT and CFD \( C_p \) start to deviate from each other on the upper surface
at the outboard bands, and at angles of attack near separation (Fig. 4.9b and 4.9c). This deviation between the WT and CFD-generated $C_p$ values results from (mostly) the CFD flow solver’s inability to capture the wing tip vortex roll-up (why the values differ for $\eta$ near 1.0) and to capture flow separation (why the values differ at high $\alpha$). Figures 4.9 and 4.10, particularly plots (b) and (c), illustrate that even though the $C_p$ values from the WT measurements and the CFD predictions (as represented by the B-spline) deviate from each other, the GP surrogates of the wind tunnel $C_p$ distribution still predict values close to the measured WT data using the CFD B-spline as the model basis function to preserve the CFD distribution’s shape; this is noticeable in regions where there are large gaps between the pressure tap locations in arc length. Thus, the GP surrogate is not restricted to match the values from the model basis function (here, $y^m(s) = \hat{C}_{p,CFD}(s_k)$), but the model basis function provides structure to the resulting WT surrogate.

![Figure 4.9: 1-D WT GP models.](image)

The plots in Fig. 4.10 depict spanwise locations and angles of attack conditions where the resulting 1-D GP mean prediction does not exactly predict all of the measured values in the WT data. The GP surrogate closely approximates the WT data, but does not interpolate through all data points. The GP model would interpolate through all data points, if there were few WT data points (increasing the number of noisy observations increases the likelihood that the GP model will need to approximate the data and not interpolate through the noisy data), and if the model basis
(a) Slat $\alpha = 21^\circ$, $\eta = 0.98$

(b) Spar $\alpha = 37^\circ$, $\eta = 0.65$

(c) Flap $\alpha = 36^\circ$, $\eta = 0.28$

Figure 4.10.: 1-D WT GP models may deviate from WT data.

function aligned with the WT data (see Fig. 4.1). The GP results for the slat in Fig. 4.10a demonstrate that the GP surrogate predictions at test locations far from WT data ($s \in [0, 0.4]$) will generally follow the CFD B-spline values, but that the hyperparameter estimates may cause the mean GP prediction to exaggerate, or over-fit the CFD B-spline. This is also evident in Fig. 4.10a on the arc length interval $s \in [0.7, 1.0]$. Thus, the “better-behaved” shape of the B-spline is not always fully transferred as in Fig. 4.1. The files containing the wind tunnel data for the Trap Wing did not have entries for pressure ports in this region (the slat cove). The raw data files did have pressure ports with $C_p = 999$ at other locations on the slat and other wing elements, which indicated that that NASA personnel reporting the data deemed that the ports were not working or the measurements were unreliable. The results in Fig. 4.10a and 4.10b indicate that the GP prediction near the leading edge ($s \approx 0.5$) may have trouble at times with large pressure fluctuations and may not perfectly predict the WT data. The GP mean prediction in Fig. 4.10a missed the WT data point at $s \approx 0.45$ as well as the location of the maximum $C_p$. The GP mean prediction in Fig. 4.10b predicts the WT data points well, but does not approximate the location of maximum $C_p$ indicated by the CFD B-spline. This may not be an issue given that the CFD B-spline’s predicted minimum $C_p$ is so much different than the WT data, but on the other hand, the B-spline and WT data on the lower surface and up to near the leading edge ($s \in [0, 0.45]$) agree so this may be a point of discussion.
for the design engineering team. All three plots in Fig. 4.10 have GP surrogates that use the CFD $C_p$ values as a basis, but the GP-predicted $C_p$ distributions do deviate in slope and value from the model basis function in regions that the surrogate predicts will best represent the WT data.

A series of 1-D GP surrogate models at the pressure port bands (tap rows) is not sufficient to represent the 2-D $C_p$ distribution in both arc length and span. However, this comparison of GP surrogates to predict $C_p$ as a function of arc length shows some of the advantages (better $C_p$ predictions between pressure ports and in regions where there are no pressure ports) and potential disadvantages (the $C_p$ of the GP surrogate model differs from measured wind tunnel $C_p$ in some cases).

### 4.4.2 Example Cross Validation for 1-D Wind Tunnel Gaussian Processes

An example assessment of the 1-D GP model, here, using a cross validation method on the flap wing element near the wing tip at $\alpha = 6^\circ$. Cross validation separates the entire data set in consideration, $\mathcal{D} = \{x, y\}$, into a training set, $\mathcal{D}^t = \{x^t, y^t\}$, and a test set, $\mathcal{D}_* = \{x_*, y_*\}$ [5, 57, 58]. The wind tunnel data set for the aerodynamic data merging when only considering the arc length variable is, $\mathcal{D} = \{x, y\} = \{s_k, C_{p,WT}(s_k)\}$. The GP model estimates the hyperparameter values using the training set, $\mathcal{D}^t = \{s^t_k, C_{p,WT}(s^t_k)\}$, and then compares the difference between the GP model predictions at the test data points, $\mathcal{D}_* = \{s_*k, C_{p,WT}(s_*k)\}$.

There are multiple strategies on how many data points to exclude from the training set, which consequently go into the test set. Two example cross validation computations here specify data as test locations for the purpose of evaluating how well the 1-D GP would do without data in a region of the airfoil, e.g., Fig. 4.10a. These examples use three and four wind tunnel data as test locations in the 1-D GP model on the flap near the wing tip $\eta = 0.98$. The red diamonds in Fig. 4.11 denote the test data, and the green circles the training data. Notice that the WT GP model predicts the shape of the data very well as long as there is an “anchor” for the WT data near $s \approx 0.02$ in
Fig. 4.11a. Figure 4.11b demonstrates that the GP model still has the same general shape of the CFD, but inverts the direction of pressure distribution when there is no anchor below \( s \approx 0.4 \). This inversion is an artifact of the WT GP hyperparameter estimates. Tests of GP models that included training data down to \( s = 0.2 \) (test data below \( s = 0.2 \)) generated the same type of inverted pressure distribution as that in Fig. 4.11b. The root mean square error (RMSE) values for the two GP models in Figs. 4.11a and 4.11b are 0.059 and 0.59, respectively. The mean absolute error (MAE) values are 0.051 and 0.43 for Figs. 4.11a and 4.11b, respectively.

### 4.4.3 Sequential Multivariate Wind Tunnel Gaussian Processes

The aim of building a surrogate model of the wind tunnel data for merging is to represent \( C_p \) values that the wind tunnel might have measured at locations - particularly in span - away from the pressure taps. This means that the surrogate model for the wind tunnel data needs to predict \( C_p \) as a function of both \( s \) and \( \eta \). This section discusses sequential GP regression modeling results for 2-D wind tunnel (WT) pressure data surrogates. Sequential GP regression is also known as online models. Most often, online GP models address time-lapsed data; here, the idea is
to include both the arc length and spanwise dimensions as input variables to the prediction. The sequential multivariate GP builds a 2-D GP by building one 1-D GP model, followed by building another 1-D GP model [59]. For this application, a first GP is built to WT data in the arc length direction at the discrete pressure port band locations, as in Section 4.4.1, and then the online approach builds another GP in the spanwise direction to the arc length GP results from the first step.

There are two main concerns with this approach: computational cost and modeling accuracy. The computational cost is a concern, because this approach requires the user to build multiple 1-D GP models to generate a single 2-D GP. The number of 1-D GPs depends on the number of pressure port bands (or pressure tap rows) and on how many 1-D GPs the user wants to build in the spanwise direction (at constant arc length values). For example, the NASA Trap Wing data supplies nine common pressure port bands for the slat, spar, and flap that align with the arc length direction. Then, in order to provide $C_p$ predictions at spanwise locations where there are no pressure tap rows, say (for example) 21 GP models are created to provide $C_p$ distributions at a given arc length as a function of span. This results in 30 individual 1-D GP models. Potential surrogate model accuracy issues from 1-D GPs in arc length would translate to the 1-D GPs in span. For example, the error in $C_p$ prediction near the leading edge of the spar in Fig. 4.10b would then be propagated into the sequential 1-D models for $C_p$ as a function of span.

The 2-D sequential GP examples shown here use the GP model setup in Table 4.6. The covariance kernels were chosen by balancing computational cost and user experience with the kernels with the idea that an engineer would not yet have investigated kernel choice for this data set (i.e., using expert judgment). Figures 4.12, 4.13, and 4.14 demonstrate the sequential GP’s capability to fit the data well for the flap element at one angle of attack; the colored surface of the GP predictions passes through or very near the red points representing the WT data in all three plots. However, the surrogates also show the sequential GP’s potential to extrapolate somewhat wildly in locations where there is no WT data to guide the surrogate. In all three plots, this is
Table 4.6: 2-D Sequential GP model characteristics

<table>
<thead>
<tr>
<th>Characteristic</th>
<th>Value / Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model basis function</td>
<td>CFD B-spline</td>
</tr>
<tr>
<td>Scale &amp; location correction</td>
<td>linear (see Eq. (4.19))</td>
</tr>
<tr>
<td>Arc length kernel</td>
<td>NN+SE+Mat</td>
</tr>
<tr>
<td>Span kernel</td>
<td>SE</td>
</tr>
<tr>
<td>$\beta$ priors</td>
<td>vague</td>
</tr>
<tr>
<td>Measurement error</td>
<td>$\sigma^2_\epsilon$</td>
</tr>
</tbody>
</table>

Figure 4.12.: Flap 2-D sequential GP surrogate at $\alpha = 21^\circ$.

evident in the blue-colored surface of the sequential GP predictions; this is somewhat counter-intuitive given the fact that the GP model uses the CFD B-spline surrogate as the model basis function and the CFD does have results in these regions and the B-spline seems to reflect these CFD-generated $C_p$ values with good accuracy. The
over-fitting / extrapolation near the flap leading at the body pod-flap joint could be due to a change in direction in WT $C_p$ data near the leading edge, and then the GP can extrapolate that curvature to somewhat extreme values. The grid lines in these
surface plots represent the locations at which the GP model is sampled for prediction values (i.e., test locations from Eq. (4.22)) after estimating the GP hyperparameter values with Eq. (4.21). The grid lines that move in the \( \eta \) direction (at constant \( s \) values) correspond to the \( s \) for the WT data locations values, but the grid lines in the \( s \) direction (at constant \( \eta \) values) do not necessarily line up with WT data points, but provide a representation of the prediction both at and between pressure bands. Many \( C_p \) plots are traditionally displayed with negative values up and positive values down (especially for the pressure distribution on an airfoil), but the surface plots here are displayed with positive values up and negative values down to show the fit quality and trends better.

Figures 4.15, 4.16, and 4.17 provide another example of over-fitting or extrapolating the predicted \( C_p \) near the body pod-slat joint. The \( C_p \) values predicted by the sequential 2-D GP model at the slat leading edge and body pod are much higher than is physically possible (e.g., areas in red boxes in Fig. 4.16.). The profile views
Figure 4.16.: Profile views of the slat 2-D sequential GP surrogate at $\alpha = 37^\circ$.

(a) $C_p$ vs. $s$, front at $\eta = 0.08$

(b) $C_p$ vs. $\eta$, front at $s = 1.0$

Figure 4.17.: Slat 2-D sequential GP surrogate with opposite view of 4.15.

in Fig. 4.16 also demonstrate the point earlier that the sequential GP $C_p$ approach is not necessarily desirable for representing the WT $C_p$ distribution. For example, the 2-D sequential GP $C_p$ predictions near the body pod and lower slat wing surface
(black box around $\hat{C}_{p,WT}(s \in [0, 0.4], \eta = y/b/2 = 0.08)$) in Fig. 4.16 seem to oscillate above and below the WT data values in between the pressure port locations. These oscillations only occur between the body pod and the first pressure port band, i.e., the sequential GP does not have WT data to “anchor” model in these regions.

The $C_p$ profile as a function of span also demonstrates that the GP predictions may have large changes really close to WT data; in this case of the flap, this happens close to—but not quite at—the wing tip $\eta = 0.82$. This spike in the GP prediction is one place where the model basis function appears to have a poor impact on the sequential 2-D GP. Figure 4.18 presents the WT data in the red symbols along with the B-spline that represents the CFD data. The color scheme is different in these plots than the rest of the surface plots in this section to distinguish the CFD B-spline results from the WT GP surrogates. Most of the time, the GP model follows the general trend of the model basis function, but not the values of the model basis function; in this case, the CFD B-spline provides the model basis function for the GP surrogate of the WT data. In this case, the upward spike in the CFD B-spline surrogate’s $C_p$ prediction near $\eta = 0.82$, which reflects how the CFD has predicted the wing tip vortex roll-up, results in a situation where the hyperparameters estimated

![Figure 4.18.: Slat 2-D CFD B-spline span profile at $\alpha = 37^\circ$.](image-url)
from maximizing the log-marginal likelihood produce a downward spike in the 2-D sequential GP model shown in Fig. 4.16b that does not seem to be supported by visual inspection of the WT data.

Appendix C provides an additional example of 2-D WT sequential GP surrogate model results on the spar; overall good representation of the WT data, but also contains regions where the GP predictions seem to incorrectly over- / under-predict the $C_p$.

In conclusion, the sequential GP method provides good approximations of the WT data at the data locations and generally in between data observations, but the potential to over- / under-predict $C_p$ values away from data points makes this a less desirable for a “hand-off” merging process.

4.4.4 Batch Multivariate Wind Tunnel Gaussian Process

This section demonstrates results of building batch 2-D Gaussian process regression modeling as a surrogate of the wind tunnel (WT) $C_p$ distribution. This method builds a batch multivariate GP surrogate, i.e., calculates the GP hyperparameters to represent the data as functions of $s$ and $\eta$ via MLE in one optimization run, as opposed to the sequential method of building multiple 1-D GP surrogates in one dimension at a time.

The batch multivariate GP uses the same equations that appear in Section 4.1. For the Trap Wing, the there are two input variables $\mathbf{x} = [s, \eta]$, so $d = 2$ in these equations. For the batch GP approach, the CFD B-spline surrogate provides predictions for the model basis function in both dimensions, i.e., $y^m(s, \eta) = \hat{C}_{p, CFD}(s, \eta)$; as before, the intent is to use the B-spline of the CFD results to help provide a better surrogate of the wind tunnel results given the sparse (particularly in the spanwise direction) location of pressure taps. The basis functions with linear scale and location
correction functions in both the arc length and span directions in Eq. (4.19) leads to the following basis function

\[
H(x)\beta = \begin{bmatrix}
1 & s_1 & \eta_1 & y^m(x_1) & y^m(x_1)s_1 & y^m(x_1)\eta_1 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
1 & s_N & \eta_N & y^m(x_N) & y^m(x_N)s_N & y^m(x_N)\eta_N \\
\end{bmatrix} \begin{bmatrix}
\beta \\
\end{bmatrix}
\]

\[
\beta = [\delta_0, \delta_1, \delta_2, \rho_0, \rho_1, \rho_2]^T.
\]

for \(N\) observations at the wind tunnel model pressure tap locations with valid \(C_P\) data. The 2-D batch multivariate GP surrogates shown here use the same kernels, model basis function, scale and location correction functions, and priors on the regression parameters \(\beta\) as the sequential approach in Table 4.6. The covariance functions are combined using Eq. (4.37) from Section 4.3.1. In other words, the covariance functions from each dimension are calculated separately and combined using both additive and multiplicative terms.

The \(C_P\) predictions from the 2-D batch GP surrogates shown via surface plots in Figures 4.19 and 4.20 indicate that the batch method does not produce the large extrapolation issues away from data points seen in the plots when using the sequential 2D GP surrogate. There is far less blue-colored (high magnitude negative value \(C_P\)) surface in Fig. 4.19 than there is in Fig. 4.12, as an example of this reduction in extrapolation issues. However, the profile view in Fig. 4.20b seems to indicate that the surrogate cannot handle the spanwise WT data distribution well; the surrogate is trending slowly downward across the entire span while the data remains fairly even until near the wing tip (see Fig. 4.13b for a reference). The results in Fig. 4.20b suggest that the GP needs additional degrees of freedom to approximate the data in the spanwise direction. The statistically significant kernels from Section 4.3.2 in modeling the flap \(C_P\) at \(\alpha = 21\) degrees are the combination of NN, RQ, SE, and Mat kernels in the arc length direction and only the noise kernel in the span direction. Figure 4.21 plots the 2-D batch GP and WT data for this kernel combination, but the GP surrogate still does not approximate the WT data in the spanwise direction extremely well. Despite the limitations, the batch surrogate predictions of the wind
tunnel $C_p$ away from data points do not have the seemingly extraneous values, or at least not as large in magnitude, when compared with the sequential GP method.

Figure 4.19.: Flap 2-D batch GP surrogate at $\alpha = 21^\circ$.

Figure 4.20.: Profile views of the flap 2-D batch GP surrogate at $\alpha = 21^\circ$. 
Additional figures for the 2-D batch GP method are in Appendix C that show similar trends with the results in this chapter. The 2-D batch GP seems to work, in a broad sense, better than the 2-D sequential GP as a surrogate of the WT data, but there are still a few regions where the accuracy is poor and/or the trends seem suspect. Therefore, this method is a more likely candidate than the sequential GP to represent the WT $C_p$ data in $s$ and $\eta$ in the “hands-off” aerodynamic data merging.
5. ADDITIVE CORRECTOR FOR 2-D SURROGATE MODEL

The motivation for the additive corrector approach is the fact that the wind tunnel data has so few different spanwise locations, which makes it difficult to build an acceptable surrogate model that uses both arc length and span as inputs. So, the additive corrector approach builds one-dimensional (1-D) Gaussian process (GP) surrogates to the WT data at the pressure bands, because this is an effective surrogate model of $C_p$ in the arc length $s$ direction. Then, the additive corrector approach uses the CFD B-spline surrogate model to provide the shape of the pressure distribution in the spanwise direction by calculating and then applying additive corrector values.

5.1 Surrogate Modeling Methodology

The additive corrector surrogate modeling methodology draws from multi-fidelity analysis in the design optimization field that combines results from engineering analysis codes of differing fidelity (and, therefore, different computational cost) [37, 39, 47, 53, 55, 60, 61]. Multi-fidelity analysis also explores the utility of a multiplicative corrector, but this work only uses the additive corrector because pressure values at or near zero can cause approximation issues for the multiplicative corrector [62]. In multi-fidelity analysis and optimization, the high-fidelity model contributes fewer data points to the combined analysis because of its relative expense compared to the low-fidelity model, but the high-fidelity model provides more accurate information than the low-fidelity model. Adapting this to the aerodynamic pressure data, the WT data and the CFD simulation results act as the high- and low-fidelity sources, respectively, because the WT data set has fewer observations in $s$ and $\eta$ compared with the CFD simulations. Application of the multi-fidelity concept does not necessarily
require that one source be of higher fidelity, i.e., the WT data is not necessarily more accurate than the CFD simulation results, but this concept does require the sources to be treated in a hierarchical fashion. Following the additive corrector concept from multi-fidelity analysis [63, 64], the value for an additive corrector term, \( C_\phi (x_k) \), at discrete high-fidelity data locations, \( x_k \), is

\[
C_\phi (x_k) = y_{hi} (x_k) - \hat{y}_{lo} (x_k).
\]

(5.1)

From several discrete \( C_\phi \) values at each \( x_k \) location, one can build a surrogate model of the additive corrector values with the idea that the additive corrector surrogate, \( \hat{C}_\phi (x) \), is easier to construct than the high fidelity surrogate, \( \hat{y}_{hi}(x) \). Then, the high-fidelity surrogate becomes the addition of the low-fidelity model plus the additive corrector surrogate

\[
\hat{y}_{hi}(x) = \hat{y}_{lo}(x) + \hat{C}_\phi (x).
\]

(5.2)

In the aerodynamic data merging context, this methodology forces the user to assume that the CFD surrogate model correctly represents the shape of the pressure distribution, and that an additive correction to this CFD-based model will approximate the WT data everywhere on the surface of the wing.

The flowchart in Fig. 5.1 illustrates the steps to generate the 2-D additive corrector surrogate for the WT data. Each step is discussed here in order, and the generic expressions in Eqs. (5.1) and (5.2) are rewritten for this aerodynamic data merging application.

Figure 5.1.: The additive corrector surrogate flowchart.

The first step in the additive corrector process in Fig. 5.1 is building 1-D GP surrogates to represent the WT data at each pressure port band, as presented in
Section 4.1. The second step is calculating the additive corrector values, $C_\phi$, from Eq. (5.1). The NASA Trap Wing wind tunnel model provided experimental data at nine pressure port bands for the slat, spar, and flap. Therefore, at each of the nine spanwise locations of the pressure tap rows, the difference between the 1-D WT GP model and the corrected CFD B-spline at a given arc length position $s_i$ becomes part of a least-squares estimation for the corrector term.

$$\arg \min_{C_\phi(s_i)} \sum_{j=1}^{\text{Numbands} = 9} \left[ \hat{C}_{p,WT}(s_i, \eta_j) - \left( \hat{C}_{p,CFD}(s_i, \eta_j) + C_\phi(s_i) \right) \right]^2.$$  (5.3)

Here, the user will specify the number of $M$ different arc length locations at which a corrector value, $C_\phi$, is computed, as illustrated in Fig. 5.1. The 1-D WT GP predictions at each pressure band do not necessarily follow the exact spanwise shape of the CFD surrogate, as Fig. 5.2 illustrates using the green symbols to indicate the values of the WT GP prediction at the spanwise location of each pressure tap row and the blue symbols to indicate value of the CFD B-spline at many spanwise locations for a given arc length position. The least-squares estimation would then try to find a single additive corrector value to minimize the sum of squared error between the CFD B-spline and the WT GP mean prediction at each of the nine pressure tap row locations. The resulting additive corrector value for the data represented in Fig. 5.2 is $C_\phi(s = 0.45) = 0.046$; here the one value of additive corrector is constant in span for this arc length location. The single additive corrector value for a given arc length position has the user assume that the CFD surrogate model correctly represents the shape of the pressure distribution in span, $\eta = y/b/2$, in an attempt to fill in the gaps between the available WT data-related predictions. As in the example of Fig. 5.2, this presumption that the CFD B-spline provides the right shape means that the “corrected” WT surrogate model does not pass through any of the associated WT values at the pressure row taps. This can lead to additional errors in the 2-D surrogate of the WT $C_p$ data. During this second step, finding values of the additive corrector term at many arc length generates a vector of $C_\phi$. The third step of the additive corrector approach uses this vector.
The third step is building the surrogate to the additive corrector values via cubic B-splines so the surrogate can generate $C_\phi$ predictions at any arc length, $\hat{C}_\phi(s)$, as demonstrated in Fig. 5.3. Figure 5.3 shows the calculated corrector value at (119) arc length locations as the large circle symbols, while surrogate model predicted values of $\hat{C}_\phi$ appear as the blue curve. B-splines work well here because they accurately represent $C_\phi$, are computationally inexpensive, and the low computational cost of generating $C_\phi$ values allows calculating a large number of $C_\phi$ values to fully characterize $C_\phi(s)$. If too few $C_\phi$ values are calculated, then $\hat{C}_\phi(s)$ may not accurately represent $C_\phi(s)$. In this work, the poor representations of $C_\phi$ manifested most often where there were too few $C_\phi$ values calculated near the leading edge of the wing elements, where there is a large change in $C_p$ values at the suction peak and the values of $C_p$ increase in magnitude, so that a relatively small difference between the 1-D WT GP prediction and the CFD B-spline prediction will require a larger absolute correction.
The last step in generating the 2-D additive corrector WT surrogate is applying Eq. (5.2) to the aerodynamic pressure data by summing the surrogate of the additive corrector values and the 2-D CFD B-spline surrogates

\[ \hat{C}_{p,WT}(s, \eta) = \hat{C}_{p,CFD}(s, \eta) + \hat{C}_\phi(s). \]  

(5.4)

Thus, the 2-D WT surrogate is a product of 1-D GPs, additive corrections to the CFD spanwise pressure distribution, and a B-spline surrogate of those corrections combined with the full 2-D CFD B-spline surrogate model.

The above described additive corrector approach requires that the user assume the CFD surrogate has the correct spanwise shape; a bold assumption given that the CFD \( C_p \) modeling is known to be off at the wing tips and at high angles of attack [3].

So, the question may be asked, ‘Why not just calculate additive corrector values between every wind tunnel data point and the CFD B-spline instead of just one for each arc length? In other words, why not generate a 2-D set of \( C_\phi \) values?’ The author investigated building a multivariate B-spline to additive corrector values at many \( s \) values, as in Fig. 5.3, and for all nine wind tunnel pressure tap rows (\( \eta_k \)), \( C_\phi(s, \eta_k) \). However, the cubic B-spline did not generate good \( C_\phi \) predictions away...
from pressure ports (taps) in the spanwise direction because nine data points in the \( \eta \) direction, at the spacing for the Trap Wing, is not sufficient to generate predictions that even closely match the flow physics in this application (extreme oscillations from over-fitting).

\[ \text{from pressure ports (taps) in the spanwise direction because nine data points in the } \eta \text{ direction, at the spacing for the Trap Wing, is not sufficient to generate predictions that even closely match the flow physics in this application (extreme oscillations from over-fitting).} \]

### 5.2 Results for Wind Tunnel Data

This section demonstrates and discusses the 2-D additive corrector surrogate for the WT data. The main (and perhaps only) advantage of the additive corrector methodology over the sequential multivariate GPs as a surrogate is the low computational cost. With this reduction in the cost, the main limitation is the potential accuracy reduction because of the least-squares-estimated additive corrector values (as documented in Section 5.1). From the outset, the author recognized this advantage and limitation, and the following figures reflect this accuracy reduction.

Figures 5.4, 5.5, and 5.6 demonstrate the additive corrector surrogate on the slat at \( \alpha = 37^\circ \). The discrepancies between the WT data and additive corrector surrogate is due largely to the least-squares-estimated additive corrector values in the spanwise direction where one corrector value is used for the entire span dimension at a given arc length position. The red symbols for WT data in Fig. 5.4 show some signs of the slat having very noisy or more fluctuation in the \( C_p \) data on the upper surface near the outboard section (\( s > 0.6 \) and \( \eta > 0.6 \)) because of separated flow. The additive corrector surrogate model reflects this by having sharp peaks in the surface plot. Figure 5.5b shows how the WT additive corrector surrogate includes the spanwise shape of the CFD results into the surrogate profile (see Fig. 4.18 for the corresponding plot of the CFD surrogate). The red symbols show the WT data in the Fig. 5.5b; for inboard locations \( \eta < 0.5 \), the 2-D surrogate model from the additive corrector approach notably under predicts the magnitude of the measured \( C_p \) from the wind tunnel, because the corrector is trying to minimize average error across the span. For outboard locations, the surface plot shows an over prediction in the magnitude...
Figure 5.4.: Slat 2-D additive corrector surrogate at $\alpha = 37^\circ$.

Figure 5.5.: Profile views of the slat 2-D additive corrector surrogate at $\alpha = 37^\circ$.

of the $C_p$ relative to the WT-measured data. The view in Fig. 5.4 best shows the sharp drop in the $C_p$ distribution at the lower surface trailing edge ($s = 0$) all along the span. This rapid change in $C_p$ is also evident in the sequential GP method, e.g.,
Fig. 4.16b, but is often more pronounced in the additive corrector surrogate because the CFD surrogate model influences this prediction of WT results more than the GP approaches. The author believes this is because the GP predictions for the sequential method are not calculated at the trailing edge, and for the batch method the 2-D GP model hyperparameter estimates are such that they do not include the large $C_p$ change from the model basis function (CFD B-spline) into the predictive model. Based upon discussions of the First AIAA CFD High-Lift Prediction Workshop, all CFD predictions showed fairly large discrepancies at the wing tips, wing element trailing edges, and generally at high angles of attack; this was particularly true for the flap [3]. Thus, the drop in the $C_p$ near $s = 0$ may be exaggerated and experimental data may clarify exactly what is going on here, provided a measurement device can be placed at the trailing edge. This might also provide hints at locations on the wing where a successful merging process would require expert input so that the wind
tunnel data might have more weight or importance in the merged $C_p$ value in some locations.

Appendix C provides additional examples of 2-D WT additive corrector surrogate model results that show the $C_p$ under-prediction on the flap and spar, particularly near the wing tips, and sometimes leading edges. The examples in the appendix are of the flap and spar at lower angles of attack, and so there are no the sharp peaks in the surface plots indicating potentially flow as in Figs. 5.4 and 5.6. However, the above trends regarding noisy data for separated flow are consistent across the wing elements at high angles of attack.
6. COMPARING WIND TUNNEL SURROGATE MODELS OVER WING GEOMETRY

This chapter discusses the results of modeling aerodynamic pressure data from wind tunnel (WT) experimental sources as a function of wing geometric variables (arc length and span, $s$ and $\eta$). These results include both qualitative and quantitative evaluations and comparisons of the additive corrector, sequential GP, and batch GP surrogate. Qualitative methods rely upon plots that demonstrate surrogate modeling and merged pressure distributions with data observations. The $L^\infty$-norm, mean absolute error (MAE), root mean square error (RMSE), and standard error of the mean (SEM) quantitative error metric equations in Table 2.1 demonstrate the surrogate modeling approximation error.

Figures of the additive corrector and Gaussian process (GP) surrogate modeling results in Chapters 4 and 5 (and Appendix C) demonstrate many of the advantages and disadvantages of each method, but some of these pros and cons are not apparent from the figures themselves. For example, the additive corrector surrogate’s advantage is low computational cost. But, this advantage comes at the cost of imposing the CFD spanwise $C_p$ shape into the WT surrogate across the entire span of the wing. This is a disadvantage when the CFD and WT data have very distinct shapes and values, leading to less accurate WT data approximation because of the least-squares-estimated additive corrector values; this is particularly evident near the wing tips, which subsequently leads to prediction error near the wing root. Another disadvantage is that the additive corrector method relies on the data being available in grids, i.e., one-dimensional (1-D) bands, which corresponds to how the pressure tap rows measure data in the wind tunnel. The sequential GP advantage is the ability to represent the data in 1-D bands. This sequential approach allows the full 2-D GP representa-
tion to be very flexible. However, this flexibility comes with costs: computationally expense, prediction extrapolation away from data points, and the need to have the data in 1-D bands. The computational cost can be excessive because each Gaussian Process model requires its own global optimization for parameter estimation. The prediction extrapolation can be an issue when the GP estimates parameters such that predictions become non-physical; one obvious example is the estimated pressure ($\hat{C}_p$) near the leading edge and wing-body junction ($((s, \eta) \approx (0.5, 0.08))$ for the flap and slat in Figs. 4.12 and 4.15, respectively, where any realistic flow could not obtain the predicted $C_p$ magnitude. The batch GP approach shows a mix of the advantages and disadvantages of the two previously discussed results. The batch GP is closer to the additive corrector in terms of low computational cost, but this cost increases more rapidly than the additive corrector with increasing the degrees of freedom through using more covariance kernels (the additive corrector computational cost increases with increasing kernel flexibility, but not as quickly). Another advantage of the batch GP is the ability to approximate the WT data and the overall shape of the pressure distribution across the entire domain of the wing geometry. This advantage contrasts with the disadvantage of the sequential GP results that can generate non-physical $C_p$ predictions (for instance, compare Figs. 4.12 and 4.19). The batch GP can also receive data in formats other than solely 1-D bands of data aligning with the independent or input variables for the surrogate (e.g., Latin hypercube or sparse grid locations of $C_p$ data could be inputs), while the additive corrector and sequential GP methods need the data to align with variables in bands (pressure port bands aligned with arc length). The batch GP disadvantage is the tendency, evident in the figures in Chapter 4, to poorly approximate the wind tunnel-based $C_p$ values at pressure port locations where the data is measured, as well as expected, or as well as the sequential method seems to predict.

The quantitative comparisons between the three WT surrogate modeling methods are made using: 1. the residuals and absolute residuals (to include value, patterns, and distribution), 2. error metrics from Table 2.1, and 3. the computational cost.
6.1 Comparing Residuals

The additive corrector, sequential (i.e., online) multivariate GP, and batch multivariate GP approaches each generate 2-D surrogate models of WT experimental data. These WT surrogate modeling approaches to build $\hat{C}_{p,WT}(x)$ each employ the calibration process in Fig. 1.2. The additive corrector method follows the process shown in Fig. 5.1. This method uses GP calibration for 1-D surrogates in arc length, and then calculates additive corrector values via least-squares estimation.

The quantitative analysis of the residuals (surrogate errors) includes plots of the residuals as a function of the independent variables, boxplots of the absolute residuals, and empirical cumulative distribution function (ECDF) plots. Residual plots and boxplots help the user see the error values and possible patterns in the residuals that should be addressed in the modeling. The ECDF plots illustrate the distribution of error to help the user compare surrogate models in their ability to represent the data. The surface plots in Sections 4.4.3, 4.4.4, 5.2, and Appendix C demonstrate some of the surrogate modeling capabilities, and an analysis of their residuals are shown here and in the appendix.

In Fig. 6.1, there are nine spanwise values from each surrogate modeling method at each of the 21 arc length values (The raw data files did have some pressure ports with $C_p = 999$ at locations on the slat, spar, and flap, which indicated that that NASA personnel reporting the data deemed that the ports were not working or the measurements were unreliable. Therefore, there are not nine $C_p$ values for all arc length locations—the average is eight per arc length location, but this discussion treats the data as though there were nine per arc length location.). Each of the nine symbols is the $C_p$ residual error averaged over all angles of attack available from the Trap Wing tests at a corresponding spanwise position of the pressure tap rows on the Trap Wing model. Similarly, Fig. 6.2 provides $C_p$ values at each of the nine spanwise positions of the pressure tap rows for the flap; because some pressure port data was removed by NASA personnel, there are just under 19 symbols on average.
Figure 6.1.: Flap WT surrogate $C_p$ residuals vs. arc length averaged over all $\alpha$.

corresponding to the $s$ pressure tap locations at each $\eta$ value for each flap surrogate model. The flap residuals are larger in magnitude near the leading edge ($s \approx 0.5$) and wing tip, as expected, because of the larger variations in absolute values of $C_p$. The additive corrector (shown using the blue symbols) consistently has higher residual values than the batch and sequential GP methods (shown in the legend as 2-D GP using green symbols and Two 1-D GPs using red symbols, respectively). The blue symbols consistently appear well below the other symbols in Fig. 6.1 along the upper surface (from $s = 0.5$ to $s = 0.85$). The batch GP has the next highest magnitude residual error values. The surrogates’ ability to approximate the WT measurements at the pressure ports makes sense based on how each surrogate is generated. The additive corrector surrogate first generates 1-D GP surrogates at each pressure port band, and then calculates additive corrector values in the spanwise direction using the CFD via least squares estimation (LSE). Imposing the CFD shape onto the WT surrogate, and calculating the additive corrector via LSE increase the WT surrogate
error. The batch GP method has higher error than the sequential GP method because the batch method needs to approximate the data over the entire design space \((s, \eta)\) using one set of optimized GP hyperparameters, while the sequential method only approximates data using multiple 1-D slices, thus giving it more degrees of freedom at increased computational cost. The sequential approach builds a GP at each pressure port band as a function of arc length and then uses these surrogates \((\hat{C}_{p,WT}(s))\) at each of the nine bands as data to approximate with 1-D GP surrogates as a function of span at discrete arc length locations \((\hat{C}_{p,WT}(s_i, \eta))\). So, the sequential GP approach tends to approximate the data better, because each GP has more freedom to approximate the data at the one 1-D section than the batch GP that has to account for all data at the same time. The error trend increasing from the sequential GP to the batch GP to the additive corrector is consistent for the slat, spar, and flap.

Figure 6.3 displays the boxplots of the absolute residuals for the surrogates plotted in Sections 4.4.3, 4.4.4, and 5.2. A boxplot is broken up into quartiles, i.e., four equal
(a) Slat at $\alpha = 37^\circ$

(b) Spar at $\alpha = 6^\circ$

(c) Flap at $\alpha = 21^\circ$

Figure 6.3.: Absolute residual boxplots for each surrogate.

Groups. 25% of the data is at or below the first quartile, $q_1$, 50% of the data is at or below the median, and 75% of the data is at or below the third quartile, $q_3$ [21]. The $q_1$, median, and $q_3$ values in the boxplots in Fig. 6.3 are shown as the bottom of the blue box, the red line in the box, and the top of the blue box, respectively. The difference between the third and first quartiles is called the interquartile range $\text{IQR} = q_3 - q_1$. The whisker that extends above the box is calculated using $q_3 + 1.5 \times \text{IQR}$, and the whisker below the box is calculated with $q_1 - 1.5 \times \text{IQR}$. Any value above or below the whiskers are considered outliers, and are marked with the red “+” symbol. The largest
absolute $C_p$ value from the NASA Trap Wing WT data for the slat pressure ports at 
$\alpha = 37^\circ$ is $\max\{|C_p|\} = 13.4$. Therefore, if the absolute residuals in Fig. 6.3a were 
changed to relative absolute residuals (absolute residuals divided by $\max\{|C_p|\}$), the 
maximum values on the vertical axis would change to 0.26. Similarly, if the absolute 
residuals of the spar and flap elements in Figs. 6.3b and 6.3c were divided by their 
respective $\max\{|C_p|\}$ values of 3.35 and 5.47 (for $\alpha = 6^\circ$ and $21^\circ$, respectively), the 
maximum values on the respective axes would be 0.27 and 0.39. Thus, the relative 
error for predicting $C_p$ on the slat is not as large the relative error for prediction $C_p$ on 
the flap, despite having large absolute residual values. The user needs to decide if the 
absolute and relative absolute residuals of the surrogates for their specific application 
is low enough for adequate representation of the $C_p$ distribution.

The additive corrector generally has larger error values than the sequential and 
batch GP when comparing the boxplots by the maximum outliers and the top whisker 
(IQR + $1.5 \times$ IQR). The batch GP consistently had lower error than the additive cor-
rector surrogate. The sequential GP had larger error for the spar surrogate compared 
with the batch GP, but lower error than the batch GP for the slat and flap surrogates, 
at these specific angles of attack. This might suggest that each element might be bet-
ter served by using a different 2D surrogate modeling approach; again, this might be 
another indication of where an expert would need to be involved in the modeling and 
merging process.

Figure 6.4 compares the absolute error between the additive corrector, sequential 
GP, and batch GP surrogates at the WT pressure port data points for the same sur-
rogates in Sections 4.4.3, 4.4.4, and 5.2 using empirical cumulative density function 
(ECDF) plots. These ECDF plots show, for a given residual error on the horizontal 
axis, how many pressure tap locations have this error or less on the vertical axis. 
ECDF plots provide a convenient method to compare different surrogate models be-
cause they not only give a relative value of the absolute error, but they also show how 
the distribution of the absolute residuals compare with other surrogates. In ECDF 
plots, surrogates with consistently lower residuals have their curve to the left of the
Figure 6.4.: Absolute residual ECDF for each surrogate.

curves of other surrogate models with higher residuals. The ECDF plots here use a semi-log plot with the x-axis transformed to the log\(_{10}\) scale.

Figure 6.4a for results at \(\alpha = 37^\circ\) shows that the additive corrector has some predictions with very low errors relative to the WT-measured \(C_p\) value, but moving to the right on the plot to count locations where the residual error increases, the curve for additive corrector begins to overtake the GP methods in the maximum error at the top right. The nearly diagonal shape for a major section of the ECDF curve for the additive corrector surrogate indicates that the distribution of the absolute residuals
for this surrogate is widely dispersed, the Fig. 6.3a boxplot also shows via the larger (taller) interquartile box and whisker locations. The sequential GP ECDF plot (the red curve in Fig. 6.4a) has a more vertical line starting from low residual values than the additive corrector in Fig. 6.4a indicating that the residuals are more concentrated at lower values (i.e., there are a larger number of observation locations where the residual is low, up to the residual value where the nearly vertical section starts). The batch GP has a nearly vertical line in residuals near the middle of its absolute residuals, showing that the batch method has fewer observation locations where the error is small as well as fewer locations where the error is large; the distribution of error for the batch method would have “lighter tails” than the additive corrector and sequential GP (similar to negative kurtosis when comparing a distribution to a normal distribution). From this figure, the author deduces that the sequential GP best represents the WT data at this flow condition for this wing element of the three methods investigated; this is also confirmed by the previous figures of residuals and boxplots.

The ECDF curves in Fig. 6.4b indicate that none of the surrogates much better than the others; all have roughly the same type of absolute residual distribution at 6° angle of attack. Figure 6.4c illustrates that the sequential GP represents the flap $C_p$ better than the other surrogates at this angle of attack, because the ECDF plot lies notably to the left of the other two curves across the range of residual errors.

The plots in Fig. 6.4 are just three of the 24 (three wing elements at eight angles of attack) ECDF plots (see Appendix C for more plots). Of the three 2-D surrogate models investigated for the WT $C_p$ distribution, none is consistently the best model for a given wing element across all angles of attack. The batch GP does not do as well as the other surrogates for representing the WT $C_p$ data on the flap element. The additive corrector does not perform better than the sequential GP, but does approximate the WT data slightly better than the batch GP, in many other cases, like the results presented in Fig. 6.4a. The surrogates for the flap generally have ECDF absolute residuals somewhat close to each other, except for a few flow conditions
near flow separation. The surrogates for the spar all seem to perform about the same across all angles of attack, similar to that found in Fig. 6.4b. The trends of the ECDF curves for the slat surrogates are different than those for the flap. The sequential GP absolute residual ECDF curves usually lie somewhere between the batch GP (usually the lowest error, or on the left in the plot) and the additive corrector (usually the highest error) curves, except after flow separation (data and surrogates for $\alpha = 37$ degrees), as in Fig. 6.4a. Based upon the non-smooth behavior of the measured $C_p$ as a function of arc length and plots of $C_p$ as a function of angle of attack for individual pressure ports (e.g., Figs. 8.1 and 8.2b), flow separation is evident in most pressure port measurements somewhere between $\alpha = 36^\circ$ and $36.2^\circ$. Interestingly, after flow separation (comparing the three wing surrogates at $\alpha = 37$ degrees), the batch GP does not perform as well as the other two surrogates (the additive corrector does about as well as the sequential GP for the spar).

The challenge here is that selection of the best 2-D WT surrogate model—which takes CFD results into account either via additive corrector and / or as a model basis function—seems to vary based on the wing element and angle of attack, if the user selects the best WT surrogate model based on $C_p$ residuals. This indicates that it would be difficult to automate this part of a merging process.

6.2 Error Metric comparison

Error metrics provide another type of assessment tool for the 2-D surrogate representations to the WT $C_p$ distribution. These metrics are the maximum error ($L^\infty$-norm), MAE, RMSE, and SEM; these metric equations appeared in Table 2.1. The reported error metric values in Table 6.1 included all residuals in the error metrics from the pressure ports and angles of attack for each wing element. For example, the $L^\infty$-norm values report the maximum absolute error between the WT $C_p$ data and the surrogate predictions for all angles of attack at all pressure ports. The $L^\infty$-norm metric shows how bad each surrogate may get because this focuses upon the largest
error between the surrogate model prediction and a measured value. The other metrics are averaging error metrics. Both SEM and RMSE metrics are included here for completeness, because when the residuals are not necessarily normally distributed the user should use SEM instead of RMSE. As discussed in Ref. [16], assessment of surrogate models should include more than one error metric. Which error metric is more appropriate to present depends on the distribution of the errors [16] (Ref. [16] compared RMSE and MAE metrics only); Gaussian error distributions, i.e., errors that follow a normal distribution, are better represented by the RMSE than the MAE, but MAE is better than RMSE when the error distribution is uniform. The error distributions from the three 2-D WT surrogate models do not follow a normal, nor a uniform distribution; thus, this work presents multiple metrics for completeness.

Table 6.1: Wind tunnel surrogate error metrics over all angles of attack using kernels NN, SE, Mat in arc length and SE in span

<table>
<thead>
<tr>
<th></th>
<th>Additive Corrector</th>
<th>Sequential GP</th>
<th>Batch GP</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L^\infty$-norm</td>
<td>3.67</td>
<td>2.75</td>
<td>3.85</td>
</tr>
<tr>
<td>Slat MAE</td>
<td>0.345</td>
<td>0.213</td>
<td>0.235</td>
</tr>
<tr>
<td></td>
<td>0.603</td>
<td>0.390</td>
<td>0.475</td>
</tr>
<tr>
<td></td>
<td>0.0211</td>
<td>0.0137</td>
<td>0.0166</td>
</tr>
<tr>
<td>$L^\infty$-norm</td>
<td>2.54</td>
<td>0.977</td>
<td>1.60</td>
</tr>
<tr>
<td>Spar MAE</td>
<td>0.193</td>
<td>0.0685</td>
<td>0.158</td>
</tr>
<tr>
<td></td>
<td>0.356</td>
<td>0.113</td>
<td>0.247</td>
</tr>
<tr>
<td></td>
<td>8.13×10^{-3}</td>
<td>2.58×10^{-3}</td>
<td>5.64×10^{-3}</td>
</tr>
<tr>
<td>$L^\infty$-norm</td>
<td>3.14</td>
<td>0.933</td>
<td>2.40</td>
</tr>
<tr>
<td>Flap MAE</td>
<td>0.191</td>
<td>0.0674</td>
<td>0.166</td>
</tr>
<tr>
<td></td>
<td>0.348</td>
<td>0.110</td>
<td>0.260</td>
</tr>
<tr>
<td></td>
<td>9.47×10^{-3}</td>
<td>2.97×10^{-3}</td>
<td>7.09×10^{-3}</td>
</tr>
</tbody>
</table>
The metric values show additive corrector surrogates almost always have the maximum absolute error \((L^\infty\)-norm), as well as the largest average error (MAE, RMSE, and SEM). The batch GP has the next lowest error metric values, and the sequential GP method has the lowest error metric values of all the surrogates. These error trends correlate nicely with the residual and error distribution plots above. It is interesting to note that the sequential GP has error metrics on the same order as the batch GP for the slat, although much lower error on the spar and flap; this reinforces the point that choosing the appropriate surrogate model to represent a set of data is problem dependent, and in this case, wing-element dependent. This is true for the additive corrector and batch GP surrogates, too, but the relative difference between surrogates in the error metrics is closer for the slat data than the spar or flap. For example, the sequential GP error metric values are about a third of the additive corrector error values for the spar and flap data, but these values are more than half of the additive corrector error values for the slat data. The above quantitative assessment of the error at the WT data locations seems to slightly favor the sequential GP method, but these metrics cannot predict how well the surrogate does away from data points. The best way to evaluate the surrogate’s ability to predict correct \(C_p\) values away from data points is through cross validation calculations of the form presented in Section 6.4.

### 6.3 Computational Cost

The computational cost is an important measure to assess how practical it might be to use one of the modeling approaches in an engineering decision-making setting, and to compare the cost / practicality of each surrogate. Table 6.2 lists the total computational cost in time to construct each type of surrogate for the WT \(C_p\) distribution on each wing element for all (8) angles of attack for which the wind tunnel measurements and CFD B-splines are available. The computational cost for the additive corrector is about an order of magnitude less than that of the GP methods. The
Table 6.2: Total 2-D wind tunnel surrogate computational cost over all angles of attack using kernels NN, SE, Mat in arc length and SE in span

<table>
<thead>
<tr>
<th></th>
<th>Additive Corrector</th>
<th>Sequential GP</th>
<th>Batch GP</th>
</tr>
</thead>
<tbody>
<tr>
<td>Slat</td>
<td>514</td>
<td>12,280</td>
<td>6,551</td>
</tr>
<tr>
<td>Spar</td>
<td>597</td>
<td>17,706</td>
<td>12,093</td>
</tr>
<tr>
<td>Flap</td>
<td>562</td>
<td>5,509</td>
<td>3,996</td>
</tr>
</tbody>
</table>

The batch GP method requires less computational time than the sequential approach, but ranges between about a third to a half of the time cost. A user may see the computational cost in Table 6.2 and the error metrics in Table 6.1, and then decide to use the surrogate that provides a combination of acceptable computational cost and low error. Another possibility would be to build a GP with fewer kernels to decrease the cost, at increased response prediction error (Table 4.4 demonstrates the cost reduction in GP modeling with fewer kernels.). This potential cost savings may inspire the user to only use one covariance kernel in each direction, assuming the resulting increase in surrogate prediction error was acceptable.

6.4 Cross Validation of 2-D Wind Tunnel Surrogates

The surrogate qualitative and quantitative evaluation in Sections 4.4 and 6.2, respectively, compare the surrogate $C_p$ predictions to the wind tunnel $C_p$ measurement used in the construction of the surrogates. In cross validation, the surrogate construction uses a subset of the available observed points (the “training set”) and the error measurement compares prediction capability of the surrogate to the remaining subset of observed data (the “test set”). This is similar to the comparisons made in Section 4.4.2 for the 1-D surrogate models of WT data. This cross validation gives the user a better idea of the surrogate’s ability to predict data away from the pro-
vided measurements or observations [5,57,58]. A cross validation case in Section 4.4.2 removed three to four data points to demonstrate the need of anchor points near the trailing edge ($s = 0.0$ and $1.0$) and at inflection points (e.g., both before and after the pressure rise near an airfoil leading edge). This section goes a step further with the cross validation and leaves out an entire pressure port band to then demonstrate the 2-D WT surrogates predictive capability without the data and the residuals at the WT data locations. This is important, because the wind tunnel data is sparse in the spanwise direction, and a comprehensive merging approach would have the ability to have a predicted value representing the WT $C_p$ distribution at any spanwise location.

Figure 6.5 shows the location of the pressure port band (i.e., pressure tap row) removed for the cross validation in this study. The CFD and wind tunnel $C_p$ values differ more near the wing tips—because of the difficulty the CFD tool has in predicting tip vortex roll up—than they differ near the wing root. Removing the pressure band

![Pressure port band](image-url)

Figure 6.5.: NASA Trap Wing planform showing the pressure port band $\eta = 0.85$ removed for cross validation.
right at the wing tip may not provide a good comparison of the three 2-D WT surrogates because all of the surrogates would probably incorrectly predict the $C_p$ values by a significant amount. The author removed the entire $\eta = 0.85$ pressure band from the data set because in the $C_p$ distribution this band lies between the well-behaved inboard $C_p$ values and the more complicated flow at the wing tip due to the vortex roll up. Removing this band may cause the 2-D WT surrogates to over-predict the pressure rise on the way to accounting for the much higher suction peak at the wing tip, and therefore, allow for a good comparison between the three different surrogates. After removing the $\eta = 0.85$ pressure band, the 2-D WT additive corrector, sequential GP, and batch GP surrogates use the rest of the data to train (or build) the respective surrogates. A comparison of predicted $C_p$ values at the $\eta = 0.85$ location to the data then helps determine the potential accuracy of the resulting surrogate models at other span locations away from the pressure tap locations. The CFD results are more disparate from the WT data on the flap wing tip than the other wing elements, so the cross validation results enumerated here are for the flap at $\alpha = 6^\circ$. The motivation for choosing the flap is that if the cross validation looks good for the most difficult part of the Trap Wing, then it should also look good for easier elements.

Figure 6.6 shows surface plot cross validation results of each WT surrogate modeling methodology employed in this dissertation, as well as red dots symbolizing the WT data used to build the surrogates (i.e., the $\eta = 0.85$ pressure band is not included in these plots). The additive corrector surrogate predictions in Fig. 6.6a do not approximate the WT data pressure well at the wing tip ($\eta = 1.0$) because of the least-squares calculations of the additive corrector values from Eq. (5.3). The sequential GP does a good job of approximating the WT data used to build the surrogate model both at the wing tip and throughout the $s$ and $\eta$ domain because 1-D surrogates in $s$ and then in $\eta$ make it much easier to fit the training data with each 1-D surrogate. The batch GP surrogate’s accuracy in predicting $C_p$ values of the training data (used to build the surrogate) at the wing tip is better than the addi-
Figure 6.6.: 2-D WT surrogates on the flap at $\alpha = 6^\circ$ constructed for cross validation.

tive corrector, but not as accurate as the sequential GP. The batch GP predictions near the inboard leading edge ($s \approx 0.5, \eta = 0.2$) do not capture the pressure rise as well as expected. As demonstrated earlier in Section 4.4, the additive corrector and batch GP surrogates seem to model general shape of the pressure distribution away from WT data (red symbols), but the sequential GP surrogate exhibits over-fitting tendencies by generating extra oscillations on the upper surface ($s > 0.5$) both near
the inboard locations ($\eta \approx 0.1$) and near the pressure port band ($\eta = 0.85$) omitted in constructing these surrogates.

The WT surrogate predictions at the “test data” pressure port band location ($\eta = 0.85$) are plotted along with CFD B-spline-predicted and WT-measured data values in Fig. 6.7. The corresponding residual errors appear in Fig. 6.8. At this

![Figure 6.7: 2-D flap WT predictions at $\eta = 0.85, \alpha = 6^\circ$.](image)

![Figure 6.8: 2-D flap WT cross validation residuals at $\eta = 0.85, \alpha = 6^\circ$.](image)
spanwise location, the CFD B-spline and WT data agree very closely for most arc length positions along the pressure band, but the 2-D WT surrogates, which did not use the WT data at this location in their construction, have trouble predicting the suction peak accurately. The additive corrector surrogate actually does the best of the three methods in predicting \( C_p \) values close to the WT data value at the suction peak, and has a smooth pressure distribution in the spanwise direction, demonstrated in Fig. 6.6a, which aligns well with the WT data. This accuracy compared with the other surrogates is somewhat surprising, because earlier demonstrations of the additive corrector method showed that this method could have issues in predicting the WT \( C_p \) values at some spanwise locations. The batch GP also has a smooth pressure distribution, as demonstrated in Fig. 6.6c, but over-predicts the suction peak at \( s \approx 0.6 \) by about 0.8 in magnitude before the predicted \( C_p \) values become closer to the WT values near the upper surface trailing edge (\( s = 1.0 \)). The batch GP probably over-predicts the suction peak here, because it is trying to “turn the corner” of the \( C_p \) distribution in the spanwise direction to capture the pressure rise at the wing tip caused by the wing tip vortices of the slat and spar impinging on the flap, as well as the flap’s own wing tip vortex. The sequential GP \( C_p \) predictions seem erratic at this spanwise location. This is because the entire 2-D method hinges on combining multiple 1-D surrogates built in the spanwise direction, and lined up next to either other; as a consequence, the whole 2-D surrogate is not always smooth nor does each 1-D GP consider the data to the left or right of it in generating the model parameters or \( C_p \) predictions. So, the sequential GP pressure distribution predictions and residuals as a function of arc length at the left out pressure band are very oscillatory.

This research compares the cross validation residuals for the three WT surrogates using the prediction sum of squares (PRESS) statistic, which is

\[
PRESS = \sum_{i=1}^{N} \left( C_{p,i} - \hat{C}_{p(-i)} \right)^2
\]  

(6.1)
for $N$ points that left out of the training set and are included in the test set. In Eq. (6.1), $\hat{C}_{p,i}^{(-i)}$ is the surrogate prediction at data point $i$ when that data point is left out $(-i)$ of the training set. Typically all data points are used at some point in the test set and correspondingly left out of the training set in cross validation. Meckesheimer et al. [5] provide a good description of selecting data for training and test sets. A cross validation of the Trap Wing $C_p$ distributions to compare all three 2-D WT surrogates using a leave-$k$-out approach for $k = 1$ and $k = 2$ (one and two data points are taken out of the training set and put in the test set) would require a computational time of about 127 and 63 computing days, respectively (using Table 6.2 as a computational cost reference). So, this research effort left one pressure tap row out to provide a window into the capability of the 2-D surrogates to represent the WT $C_p$ distribution away from the pressure taps. The additive corrector, sequential GP, and batch GP PRESS statistics are 1.099, 2.326, and 3.038, respectively. A complete cross validation study is needed before drawing a strong conclusion based on the PRESS metrics.

### 6.5 Summary of Modeling Comparison in Wing Geometry

Each of the considered surrogate modeling methods for the WT data has its advantages and disadvantages. Table 6.3 provides a good summary of the 2-D WT surrogate modeling trends for accuracy of modeling the WT data, general ability to model the flow physics, and the required computational time. Generally, the addi-

<table>
<thead>
<tr>
<th></th>
<th>WT data accuracy</th>
<th>Modeling flow physics accuracy</th>
<th>Computational cost</th>
</tr>
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<tbody>
<tr>
<td>Most</td>
<td>Seq. GP</td>
<td>Batch GP</td>
<td>Seq. GP</td>
</tr>
</tbody>
</table>

Table 6.3: 2-D Wind tunnel surrogate ordering
tive corrector does not approximate the WT data as accurately as the GP methods, because it relies on the assumption that the CFD B-spline surrogate has the correct spanwise shape, and then calculates a least-squares estimate of the additive corrector to get as close an estimate of the WT data as possible. Because the CFD simulation results had trouble modeling the $C_p$ near the wing tips due to wing tip vortices as well as $C_p$ values at high angles of attack, the additive corrector assumption introduces this modeling error into the 2-D WT additive corrector surrogate. On the other hand, the sequential GP provides relatively good approximations of the WT data at the observation locations (pressure ports), but this surrogate has some over-fitting or extrapolation issues near the wing tip and inboard spanwise location because there are no WT data points to “anchor” the 1-D GPs at some specific arc length locations ($s \in [0.5, 0.7]$, in Fig. 4.17 is a good illustration of this). The batch GP surrogate does a good job of approximating the WT data and following the general trend of the $C_p$ distributions demonstrated by the WT data as well as the CFD results. In summary, the order of qualitative WT data approximation accuracy for the three surrogates from least to most accurate is the additive corrector, then the batch GP surrogate, and then the sequential GP.

The additive corrector surrogate model is the least expensive in computational time followed by the batch GP and then the sequential GP. The batch GP computational cost can vary significantly depending on the number and type of kernels in use. Without a covariance kernel (besides the measurement noise variance kernel), the batch GP has lower computational cost than the additive corrector, but this increases to about an order to two orders of magnitude greater than the additive corrector when multiple covariance kernels are employed. The sequential GP model’s cost also varies with the number and type of kernels, but computational cost for the sequential GP is always greater than the batch GP approach, but the difference is smaller when each GP employs many covariance kernels.

The correct selection of surrogate models (or combination of surrogates [65–67]) depends on the surrogate’s ability to represent the physics, approximate the data (low
residuals), and have reasonable computational cost. The comparison results in this chapter illustrate that no single model works best for all wing elements in all flow conditions. Some maximum error values might preclude using the 2-D WT surrogate models either as a “merged result” in its own right, or as a representation of the WT data in a subsequent merging step. This means that some expert oversight is still needed for using these WT surrogates in an aerodynamic pressure data merging approach.
7. MERGING METHODS

In Chapter 1, Fig. 1.1 illustrated a notional flow chart for the merging process. This process would combine information from the CFD-calculated pressure distribution and from the wind tunnel measurements of pressure to provide a “best” estimate of $C_p$ at any combination of arc length and spanwise location on the wing. To provide this estimate at any arc length and spanwise location, the merging requires surrogate models because the CFD provides wing surface pressure values at discrete grid locations and the wind tunnel provides surface pressure values at the discrete (and far more sparse) pressure tap locations on the model. Because of the sparsity of data from the wind tunnel, the construction of the wind tunnel surrogates leveraged information from the CFD pressure distribution, so these 2-D surrogate models of the WT $C_p$ distribution could provide “merged” $C_p$ values on their own. However, based on observations noted in preceding chapters, there are locations on the wing where higher “belief” should be provided to one information source over another, so an additional step that uses user-defined belief weights provides another means of computing a merged $C_p$ distribution.

7.1 The Calibration Process: A Merging Perspective

As Section 1.2 described when introducing the merging process, the GP surrogate modeling for representing the WT $C_p$ distributions allows the user to leverage data sources that are rich in information to calibrate or inform the surrogate models of information-scarce data sources. This should generally allow hyperparameter estimates to better represent the scarce data source. So, the CFD surrogate calibrates the WT surrogate with the intent to improve WT GP predictions where few or no WT measurements exist. The calibration process (within the merging process, de-
picted in Fig. 1.1) generates the WT surrogate model, $\hat{C}_{p,WT}(x)$ by using both the CFD surrogate-predicted $C_p$ values at the WT pressure port locations, $\hat{C}_{p,CFD}(x_k)$, and the WT $C_p$ measurements at the pressure ports, $C_{p,WT}(x_k)$. Figure 1.2 depicts three different calibration methods for the two dimensions in this work (normalized arc length and span): 1) two one-dimensional Gaussian processes (1-D GPs) in series, i.e., the sequential 2-D GP, 2) a set of 1-D GPs in arc length followed by an additive corrector, and 3) a 2-D batch multivariate GP, i.e., computed all at once.

Because the calibration process takes data from both sources, this may be a sufficient merging of the two data sources when the data values align or are very close, as in Fig. 4.9a. Generally, the desire to match the measured WT $C_p$ values in the calibration approaches carries the inference that the WT values are more accurate or have more weight in the merging, if these WT GP models are viewed as the entire merging process. The additive corrector approach, which would treat the WT values as most important in the 1-D GP surrogates, then compromises between the WT and CFD values when trying to minimize the difference in $C_p$ predictions along the spanwise direction. This compromise in the additive corrector essentially gives higher weight to the shape of the CFD $C_p$ distribution but not necessarily to the value of either $C_p$ distribution. Because of this, the merging process may require an additional step when the engineer believes the true pressure distribution is aligned with one of the two surrogate models’ predictions, or somewhere in between.

7.2 Merging via Belief Weights

This section presents data merging using a weighted-sum approach from the perspective that the calibrated WT GP surrogate does not represent the engineer-perceived true pressure distribution, so an additional step is required to merge the CFD and WT two surrogate models. This contrasts with the viewpoint mentioned in Section 7.1 where the engineer believes the WT surrogate represents the true pressure distribution, so generating the WT surrogate model is a sufficient merging. If both
the WT and CFD surrogates had predicted distributions of error (or uncertainty), then the data could have been merged using the predicted means and variances [37].

Here, the author used a straightforward weighted-sum approach to merge the two surrogate models. This method is also called a weighted average in some literature [65–67]. The final 2-D merged pressure distribution combines the 2-D CFD B-spline and WT surrogates using a weighted sum of the form

\[ C_{p,\text{merged}}(s, \eta) = w_1(s, \eta)\hat{C}_{p,\text{WT}}(s, \eta) + w_2(s, \eta)\hat{C}_{p,\text{CFD}}(s, \eta). \quad (7.1) \]

The WT and CFD belief weights, \( w_1 \) and \( w_2 \), respectively, reflect the engineer’s relative belief as to which surrogate best represents the true distribution. Ullman presents a method to determine belief weights using a belief map based on user knowledge and confidence levels [68]. Other methods of developing the weights can be based on the error of each surrogate model [66], or the deviation of each surrogate’s prediction from the average prediction of an ensemble of surrogates [67]. Regardless of the method to develop the belief weights, for the aerodynamic data merging they must
1) sum to unity, and 2) be \( C^0 \) continuous (ensures that \( C_{p,\text{merged}} \) does not have extraneous discontinuities). The weights can vary as a function of each variable independently. The merging through Eq. (7.1) is the final step in the merging process from Fig. 1.1.

Figure 7.1 provides comparisons of \( C_p \) values at the same wing elements, spanwise locations and angle of attack values as the plots in Fig. 4.9. The weighted sum values used for the additional merging step in these examples appears in Fig. 7.2. In these plots, the 2-D surrogate model of the wind tunnel \( C_p \) distribution uses the additive corrector approach (hence, the WT \( C_\phi \) 2-D label in the legend). At the spanwise locations in Fig. 7.1a, 7.1b, and 7.1c, the 1-D GP mean prediction of \( C_p \) (the dashed green line) matches the measured wind tunnel data (the green symbols) well, but the resulting 2-D additive corrector estimate of \( C_p \) is not always close to the WT data, or to the CFD surrogate prediction. The GP mean prediction approximates the WT data well, but the 2-D additive corrector estimate is not always close to the WT or CFD data. This discrepancy is because the least-squares calculation of each
Figure 7.1: $C_{p,\text{merged}}$ 1-D distribution slices using the 2-D additive corrector WT models (same wing elements, $\eta$ locations, and $\alpha$ as in Fig. 4.9a).
	headvise{additive corrector $C_\phi$ in Eq. (5.3) minimizes the difference between the 1-D WT GP predictions and the sum of the CFD B-spline and $C_\phi$ at all pressure port bands (a.k.a. pressure tap rows) at one specific arc length; there is no variation in corrector value along the span of the wing. The least squares equation is repeated here to illustrate}

$$\arg \min_{C_\phi(s_i)} \sum_{j=1}^{\text{Numbands}} \left[ \hat{C}_{p,WT}(s_i, \eta_j) - \left( \hat{C}_{p,CFD}(s_i, \eta_j) + C_\phi(s_i) \right) \right]^2. \quad (7.2)$$
So, one additive corrector value at arc length \( s_i \) is calculated using all nine pressure port bands. Figure 7.1a helps illustrate the point that even when the CFD, WT data, and 1-D WT GP surrogate are closely aligned at a given spanwise location, the additive corrector adjustment across the entire wing span may cause the 2-D additive corrector surrogate, \( \hat{C}_{p,WT}(s, \eta) \), prediction to imperfectly represent the WT data at the pressure port band where WT data is available. The 1-D GP will approximate the WT data at each pressure port band, but the additive corrector averages out the deviations between CFD and WT surrogates across all bands, as in Fig. 7.1a. The red dot-dash lines in Fig. 7.1 are the 2-D additive corrector predictions at the respective pressure port bands.

Now, to demonstrate the belief-weighted merging step, the CFD B-spline surrogate represents the CFD \( C_p \) distribution and (here) the 2-D WT additive corrector surrogate represents the wind tunnel \( C_p \) distribution. The engineer desiring a merged value must specify (or perhaps obtain from a group of experts) how the belief weights might vary over the surface of the wing. For instance, limitations in the ability of CFD tools to predict separated flow might lead to a decreased belief in the CFD-predicted \( C_p \) values near the upper surface trailing edge of the wing elements. Consideration of the wing tip vortex might also lead to a higher belief weight near the wing tips.

![Figure 7.2.: Merging belief weights](image-url)
Perhaps in regions far from pressure taps (or where pressure tap data is deemed to be poor—like the “999” entries for $C_p$ in some of the Trap Wing wind tunnel data), the CFD results might receive higher weight. Using the belief weight variation as a function of arc length presented in Fig. 7.2 and constant in span, the final 2-D merged pressure distribution, the solid black line, combined the 2-D CFD and WT surrogates using the weighted sum approach in Eq. (7.1).

The merged $C_p$ values, after using the belief weights, in Fig. 7.2 show a few potentially concerning issues. For instance, on the slat at $\alpha = 37^\circ$ and at $\eta = 0.17$, both the 1-D GP mean prediction of the WT and the CFD B-spline at this spanwise location appear quite similar, but the belief weight merged results for $C_p$ differ greatly from both of the original sources. In Fig. 7.1a, this is particularly evident for the section of arc length between about 0.5 and 0.8; similar discrepancies appear at other arc lengths. This is an artifact of using the additive corrector approach for the 2-D WT surrogate model, which drives the merged value to a poor value because—at this location—the 2-D additive corrector surrogate is a poor surrogate. The merged value does lie between the red “dot-dash” line and the small blue symbols, indicating that the belief weight merging does result in a value between the two surrogates. Figure 7.1b for the spar at $\alpha = 24^\circ$ and at $\eta = 0.98$, also shows that the solid black line representing the belief weight merged $C_p$ lies between the 2-D WT additive corrector and the B-spline CFD surrogates, but again the additive corrector approach does not provide a good surrogate near the wing tip. Fig. 7.1c also shows similar results. A user may see the 2-D WT additive corrector surrogates in Fig. 7.1 and correctly assume that they may as well just use the WT data along those pressure port bands. However, some reasons to use surrogates with an appropriate amount of error include 1) the ability to generate merged $C_p$ predictions in a more automated fashion with less user interaction, 2) surrogates provide prediction estimates at any location in the design space, and 3) it is important to evaluate multiple surrogates because specific problem physics may conducive to using one surrogate, or a set of
surrogates, over another. Using the 2-D additive corrector approach as a precursor to the belief weight merging, however, does not appear to be a good option.

Figure 7.3 shows 1-D slices of the 2-D sequential and batch GP surrogate models at the $\eta = 0.17$ pressure port band; these surrogates and the subsequent belief-weighted merged $C_p$ distributions are much closer to the actual WT data and CFD B-spline values. As a reminder, building the 2-D sequential GP requires generating a 1-D GP

![Figure 7.3: $C_{p,\text{merged}}$ 1-D distribution slices using the 2-D GP models for the slat at $\alpha = 37^\circ$, $\eta = 0.17$.](image)

at each pressure port band in the arc length direction, and then generating another set of 1-D GPs in the spanwise direction that approximate the $C_p$ predictions of the 1-D GPs in the first step. Thus, the fact that the sequential 2-D GP goes through the WT data in Fig. 7.3a is unsurprising; the belief weighted merged $C_p$, then lies between the 2-D WT sequential GP and the CFD B-spline surrogate. The 2-D batch GP is generated using an all-at-once approach; i.e., there is only one estimation of hyperparameters for the entire design space. This requires that a few hyperparameters enable the GP surrogate to approximate the data at any location in $s$ or $\eta$. The 1-D slice of the batch GP results in Fig. 7.3b are not perfectly aligned with the WT data, but are sufficiently close, and much closer than the 2-D additive corrector surrogate in
Fig. 7.1a. Here, the belief-weight merged result again provides the weighted average between the 2-D WT surrogate and the CFD surrogate as governed by Fig. 7.1a.

Figures 7.2 and 7.4a provide other examples of possible belief weights the engineer could use. The author chose these belief weights as examples in the merging process. The weights in Fig. 7.2 reflect the engineer’s belief that the WT surrogate perfectly represents the actual flow conditions at the lower and upper surface trailing edges (s = 0 and 1, respectively), while the CFD surrogate contributes more information near the leading edge (s = 0.5), which resulted in the merged distributions demonstrated in Fig. 7.1. The weights in Fig. 7.4a resulted in the merged distribution in Fig. 7.4b, and reflect the engineer’s belief that the WT surrogate is 20% accurate in representing the actual flow physics while the CFD surrogate is 80% accurate. The results in Fig. 7.4b are the same as in Fig. 7.1a, except for the change in belief weights. The change in the merged $C_p$ distribution is most noticeably different between arc length values of 0.5 to 1.0 (i.e., between the upper surface leading edge and trailing edge).

The above figures showing additive corrector surrogates and the merged $C_p$ distributions indicate that this surrogate modeling methodology might not always be the
best option, in terms of modeling accuracy. The $C_p$ slices of the sequential and batch GP surrogates for the slat at $\eta = 0.17$ in Fig. 7.3 indicated that the other surrogates in this thesis provide reasonable alternatives to the additive corrector model, and these might lead to a better merged $C_p$ value. The following figures compare the surrogate models and merged data set on the slat at different spanwise locations than shown above; the comparisons are at $\eta = \{0.80, 0.85\}$, where $\eta = 0.80$ is a spanwise location in between pressure port bands so no actual WT data exists at this location, and where $\eta = 0.85$ is at a pressure port band. The reason for evaluating the surrogates at a spanwise location without WT data is to demonstrate how well the 2-D WT surrogate operates at locations on the wing where there is no data. Also, the additive corrector surrogate in Fig. 7.5 (remember that the 2-D additive corrector surrogate uses the CFD $C_p$ distribution shape in the spanwise direction) shows that the CFD results have an abrupt rise and fall in the slat $C_p$ just after $\eta = 0.80$ for $\alpha = 37^\circ$. Therefore, the author chose to evaluate the surrogates and merged pressure

Figure 7.5.: Slat 2-D additive corrector surrogate spanwise profile view at $\alpha = 37^\circ$. 
distributions around this sharp $C_p$ change. Figure 7.5 is a repeat of Fig. 5.5, and is a spanwise profile view of the 2-D WT additive corrector surrogate for the slat at $\alpha = 37^\circ$. Figure 7.5 demonstrates some of the discrepancies between the additive corrector surrogate model (surface) and the WT data (red dots), which occur near (or at) the leading edge.

The belief-weight merged $C_p$ distribution in Fig. 7.6a is much closer to the wind tunnel surrogate, in general. Near the leading edge, where the assigned belief weights give more importance to the CFD solution (see Fig. 7.2), there is a larger difference between the red “dot-dash” line and the solid black line. Fig. 7.6b once again indicates that the method does not necessarily approximate the WT data due to the least-squares calculations of the additive corrector values ($C_{\phi}$). Figure 7.6b shows that for the slat at this angle of attack, the WT $C_{\phi}$ 2-D surrogate predicts values much closer to the WT data $C_p$ at this spanwise position, with the exception of the arc length values from just below $s = 0.6$ to the trailing edge. As a result, the belief weight merging leads to a $C_p$ prediction that lies between the 2-D WT surrogate and the CFD B-spline, and the poor performance of the additive corrector surrogate at this
spanwise location for the upper surface leads to poor performance of the belief-weight merged prediction.

Figures 7.7 and 7.8 show similar comparisons of $C_p$ distributions; here, however, these figures use the 2-D sequential GP surrogate model for the wind tunnel data (Fig. 7.7) and the 2-D batch GP surrogate model for the wind tunnel data. These other 2-D surrogate models for the wind tunnel $C_p$ distribution showed promise in earlier comparison, so the belief-weight merged $C_p$ values using these surrogate models should also show improvement over using the additive corrector 2-D surrogate for the wind tunnel $C_p$. These figures are for the slat wing element at the same spanwise locations as the comparison plots in Fig. 7.6 that used the additive corrector surrogate.

Figures 7.6a, 7.7a, and 7.8a have no WT data for comparison, so these plots the

![Graphs showing Cp distributions](image)

Figure 7.7.: $C_{p,merged}$ 1-D distribution slices of the slat at $\alpha = 37^\circ$ using the 2-D sequential GP surrogate with the belief weights from Fig. 7.2.

$C_p$ result that would come from the belief-weighted merging process. When the 2-D surrogate model of the WT distributions in Figs. 7.6b, 7.7b, and 7.8b does a good job representing the WT data, then the belief-weighted merging provides a believable weighted average $C_p$ value that lies between the CFD and WT values.
Figure 7.8.: $C_{p,merged}$ 1-D distribution slices of the slat at $\alpha = 37^\circ$ using the 2-D batch GP surrogate with the belief weights from Fig. 7.2.

The results in this section demonstrate that the better the 2-D WT surrogate modeling, the better the merging; this is evident by comparing the additive corrector, sequential GP, and batch GP methods in Figs. 7.1a and 7.3 or Figs. 7.6, 7.7, and 7.8. The belief weights provide a slightly more structured way to think about merging than just having a group of engineers discuss what data source they believe; the process would make them describe where on the wing they believe one source over the other and to quantify this belief.

### 7.3 Merging Summary

There are two different perspectives of merging for the aerodynamic data: 1) by using the CFD B-spline as a model basis function for the various Gaussian Process models of the wind tunnel data, these GP surrogates themselves represent a merging of the data, and 2) even with the CFD B-spline providing the model basis function for the WT surrogates, the 2-D surrogate only represents the WT data and there may be locations on the wing where the difference in predicted $C_p$ values from the
wind tunnel surrogates and the CFD surrogate need to be combined in some way to give the best merged estimate. The first perspective with the GP surrogate of the WT using the CFD B-spline as a model basis function is more readily automated, while the second approach requires additional interaction with users or experts to determine the weighting factor values and how they vary in span and arc length. The belief-weight merging provides a combination of the two estimates, and this more likely reflects “true” conditions.

The merging surrogates in this chapter demonstrate (and reinforce the conclusions from Chapter 6) that the additive corrector is not the best surrogate for modeling the WT data, in spite of the low computational cost. However, if computational cost was the major factor, then the additive corrector may be an acceptable starting point for design and analysis. The sequential GP surrogates represents the available wind tunnel data well, but the tendency to over-fit or poorly extrapolate the pressure distributions near the inboard and wing tip (shown through surface plots in Section 4.4), as well as the high computational cost to estimate all of the hyperparameters via global optimization leads the author to recommend the batch GP as the surrogate of choice for the best overall performance in modeling the WT data accurately at somewhat lower computational cost.

Following the approach of building two separate surrogates for the WT and CFD data sources, then assigning belief weights to compute a final merging takes more input from the user and / or additional experts. However, this might provide the best possible merging results with a bit more structure than a more ad hoc approach. The cost with these benefits are engineer time (including the learning curve on understanding surrogates), computational time in constructing the surrogates, and surrogate accuracy (surrogates introduce error into data predictions).
8. PRESSURE OVER ANGLE OF ATTACK

In the previous chapters, the surrogate modeling and merging processes focused upon the $C_p$ distribution as a function of the location on the wing; however, data in most studies—like that of the Trap Wing for the High-Lift Prediction Workshop—also consider different flow or flight conditions. The Trap Wing study also investigated changes in $C_p$ as a function of angle of attack, so this could be considered another important independent variable for the surrogates and merging process. The wind tunnel (WT) data usually has a richer set of information than the CFD in the angle of attack variable because of the relative ease of generating data by varying the angle of attack of a WT model compared with the computational cost of generating CFD solutions at each flight condition. This wealth of information from the WT compared with CFD in angle of attack is opposite in that the wind tunnel model is quite sparse of measurements in the arc length and span (wing geometry) variables. Investigations into surrogate modeling methods to represent $C_p$ as a function of $\alpha$ indicate that B-splines, singular value decomposition (SVD), and Gaussian Processes with model basis functions do not provide adequate surrogates. B-splines have a tendency to over-fit noisy data. SVD introduces pressure distribution discontinuities into the model that do not exist in the data. Also, generating good model basis functions is difficult for Gaussian processes with model basis functions, at least for the given data from the Trap Wing study. Therefore, this research effort used Gaussian process (GP) modeling with no model basis function (i.e., using the GP regression equations from Section 4.1) as the only potentially viable surrogate for $C_p$ as a function of $\alpha$.

Ideally, generating surrogate models of $C_p(s, \eta, \alpha)$ for both CFD and WT data sources would enable merging data in all three variables; this would provide the most flexible and easiest methodology to use the merging process. However, the $C_p$ data in $s$ and $\eta$ is extensive for CFD, but limited in $\alpha$, so no surrogate can be built to all three
input variables simultaneously for CFD. As seen in earlier chapters, the WT data has limited \( C_p \) data in \( s \) and \( \eta \), so constructing \( \hat{C}_p(s, \eta) \) via a Gaussian Process must first have a CFD surrogate as the model basis function. Thus, the WT \( \hat{C}_{p,WT}(s, \eta, \alpha) \) would need some sort of sequential surrogate modeling that first builds \( \hat{C}_{p,WT}(s, \eta) \), and then somehow builds a subsequent surrogate to introduce \( \alpha \) as the additional independent variable.

One significant challenge in building a surrogate model that represents how \( C_p \) changes as a function of angle of attack is that the resulting function, at least when trying to build a surrogate for the wind tunnel model, must include discontinuities associated with flow separation. For instance, the pressure on the upper surface of a wing element may vary relatively smoothly with angle of attack until a sufficiently high (or also, as the data suggests, sufficiently low) \( \alpha \) when the flow will separate. This appears in the data associated with a pressure tap location as the \( C_p \) smoothly changes value for several consecutive \( \alpha \) values, then at the next \( \alpha \) in the data, the \( C_p \) value has changed substantially. Because of this, research into various modeling methods to approximate \( C^0 \) discontinuities indicated treed Gaussian processes (GPs) [24,51], GP product-of-experts models [22,69–71], and deep GP models [26,50,72] were viable options. Surrogate modeling of the pressure distribution as a function of angle of attack used Gaussian process (GP) regression with a product-of-experts approach. Specifically, this research used product of experts (PoE) and generalized product of experts (gPoE) methods outlined by Cao and Fleet [22], and Deisenroth and Ng [69].

8.1 Methodology

8.1.1 Data Preprocessing

The effort here built the Trap Wing WT data surrogate model in the angle of attack dimension using the following steps: 1) download the WT data from the HiLiftPW-1 website [2] and save the data in a format easily accessible for surrogate modeling, 2) identify and remove pressure port data that NASA experts identified
as outliers (these appear as locations where \( C_p = 999 \)), 3) split the data up into sections where the flow separation occurs using a Gaussian mixture model to handle the associated discontinuities, 4) build a GP regression model to each data section (the individual “expert” models), and 5) combine each GP expert model into the complete GP surrogate model using the PoE approach to get one \( \hat{C}_p(\alpha) \) that works across the range of \( \alpha \) present in the data.

### 8.1.2 Challenges

The first two steps were straightforward preprocessing steps. The fourth step required building a GP regression model to the data, which was straightforward given past experience with building 1-D GP models when the independent variable was a direction associated with the wing geometry (like arc length). Steps three and five were more complicated. Building a GP regression model for \( \alpha \) values where the flow is attached and a different GP regression model for \( \alpha \) values where the flow is separated requires dividing the data. However, the flow did not separate at the same angle of attack for all pressure ports, so picking one angle at which to divide the flow-separated data from the flow-attached data would not provide as clean a split, theoretically, as a method to estimate which data belongs to the non-separated and separated flow groups. Also, some pressure ports had two apparent flow separation points in \( \alpha \), one near zero degrees angle of attack (\( \alpha = 0^\circ \)) where flow separates for pressure ports and remains separated for \( \alpha < 0^\circ \), and another near \( \alpha = 36^\circ \) where flow separates and remains separated for \( \alpha > 36^\circ \). Figure 8.1 is a plot of pressure coefficient as a function of angle of attack for the spar element measured by a pressure tap at \( s = 0.59 \) and \( \eta = 0.18 \); the plot here displays the discontinuities in \( C_p \) as a function of \( \alpha \). The main complication with step five is determining how to combine GP models (GP experts) from each data section into one surrogate model over the entire domain.
8.1.3 Gaussian Process without a Model Basis

The general Bayesian calibration model, from Kennedy and O’Hagan, is the Gaussian process (GP) regression model of the form

$$y(x) = \rho(x) y^m(x) + \delta(x) + \epsilon = f(x) + \epsilon$$  \hspace{1cm} (8.1)$$

where $y$ is the observation at independent variable values $x$, $\rho$ and $\delta$ are the scale and location correction functions, $y^m$ is the model basis function, $\epsilon$ is the error model (assumed independent and identically distributed measurement noise, $\epsilon \sim \mathcal{N}(0, \sigma_n^2)$), and $f$ is the actual process. However, in modeling the wind tunnel $C_p(\alpha)$, there is no model basis function because the CFD simulation results are so sparse in angle of attack, there’s no good way to build a B-spline (or other) surrogate that includes $\alpha$ as an independent variable. So, without a basis function, Eq. (8.1) reduces to

$$y(x_i) = \delta(x_i) + \epsilon_i.$$  \hspace{1cm} (8.2)$$

This is the same as Eq. (4.1). In Eq. (8.2) $y$ are noisy observations (i.e., measurement uncertainty) of the actual process, $f$ (The NASA Trap Wing WT data files
provide uncertainty values on the wind tunnel flow conditions, but not on the pressure measurements.). These observations are the wind tunnel pressure measurements at discrete angles of attack, \( y(x) = C_p(\alpha) \). The GP model uses the observations to estimate the GP model hyperparameters, and then the GP regression model predicts \( C_p \) values as a function of \( \alpha \). The GP model is the same as that in Sections 4.1 and 4.1.1, and the GP, which comprises a mean function \( \mu \) and a covariance function \( K \), can represent the actual process, which itself is a function of the input or independent variables \( x \).

\[
f(x) \sim \mathcal{GP}(\mu, K)
\]  

(8.3)

The GP model hyperparameters, \( \theta \), define the kernel and the measurement noise characteristics. The \( \theta \) estimation equations and the \( C_p(\alpha) \) (i.e., actual process) prediction equations are given in Section 4.1.1.

If the \( x \) domain is divided into sections to model discontinuous behavior in the actual process, e.g., flow separation, then GP regression models can be built using the observations in each section and combined with the product-of-experts approach in Section 8.1.5.

### 8.1.4 Gaussian Mixture Modeling

This section discusses how the author divided the data points for pressure coefficient versus angle of attack into clusters using Gaussian mixture models (GMM) and why the data necessitated using a GMM approach.

The aerodynamic pressure data are split into clusters depending on whether the data corresponds to the angle of attack before or after flow separation occurs. The angle of attack at which flow separation occurs is noisy. At a given pressure port location, as the angle of attack increases and the boundary layer separates, the value of the pressure coefficient makes an almost discontinuous jump; then, as the angle of attack increases further, the flow may reattach leading to another nearly discontinuous jump in \( C_p \) back to levels that would be near to those before the initial separation.
As a result, making a distinct statement about an angle at which flow separates is essentially impossible; therefore, the value of $\alpha$ associated with flow separation is noisy. GMM probabilistically calculates whether a data observation belongs to different clusters; here, whether a $C_p$ value near a flow separation angle of attack belongs to attached or separated flow clusters.

Figure 8.2 shows the pressure data as a function of angle of attack for two pressure ports on the slat wing tip ($\eta = 0.98$). Figure 8.2a indicates pressure port locations on the slat cross section associated with the wing tip pressure band and highlights the pressure ports with pressure data plotted in Figs. 8.2b and 8.2c. Figure 8.2b demonstrates two different possible flow separation regions as a function of angle of attack; one seems to occur near zero ($0^\circ$) and another definitely occurs near $\alpha = 36^\circ$. The plot has lines drawn connecting the discrete measurement data to show that the flow separation around $36^\circ$ is noisy; the pressure data shows separated flow for the wing at $36.12^\circ$, but not at $36.16^\circ$, and then the data indicates the flow remains separated for all subsequent angles of attack. The flow separation around $36^\circ$ is not evident from the pressure data at all ports, as in Fig. 8.2c where there is a change in slope of the $C_p$ vs $\alpha$ curve, but not a significant jump. However, ports that do demonstrate the flow separation behavior around $36^\circ$ consistently have separated flow at $36.12^\circ$, but not at $36.16^\circ$, and then separated flow for all subsequent angles of attack. In that case, the user could index each angle of attack and attach identifiers to specify whether the associated data is for separated or non-separated flow. On the other hand, the angle of attack at which the flow separated near $\alpha = 0^\circ$ varied from port to port by roughly $\pm0.5^\circ$. So, the author used Gaussian mixture modeling (GMM) to probabilistically “assign” data points to attached or separated flow clusters, and then decided to use this clustering algorithm for the flow separation at both $0^\circ$ and $36^\circ$ angles of attack. Constructing the surrogate for $C_p$ as a function of $\alpha$ needs this distinction between whether the WT data is part of the attached flow or separated flow cluster.
The GMM clustering separates data into each cluster based on probabilities that the data points come from a “source” that produced nearby data. All of the $C_p$ data here is from the wind tunnel testing; in the GMM context, the source is either attached flow or separated flow. The data-cluster identity (DCI) probabilities are calculated through either maximum likelihood estimation (MLE) or maximum a posteriori (MAP) parameter estimates. The MAP calculations require prior parameter probabilities for Bayesian inference, but no priors exist for the data in this effort, so the author estimated the parameter values via MLE. Direct maximization of the likelihood function is not possible because the calculations are nonlinear. Therefore, the
The author calculated the parameters using the well-established estimation-maximization (EM) algorithm with an open-source code [73] (this is not the same as maximizing the log marginal likelihood in Section 4.1.1).

The following Gaussian mixture model (GMM) mathematical details come from Ref. [70]. The GMM is a weighted sum of $L$ Gaussian distributions of the form

$$ p(x|\lambda) = \sum_{i=1}^{L} w_i g(x|\mu_i, \Sigma_i) \quad (8.4) $$

where $w_i$, $x$, and $g(x|\mu_i, \Sigma_i)$ are the weights, $d$-dimensional input, and Gaussian distributions, respectively. The weights $w_i$ must sum to unity. These parameters are represented as

$$ \lambda = \{ w_i, \mu_i, \Sigma_i \} \quad i = 1, \ldots, L \quad (8.5) $$

Each Gaussian is of the form

$$ g(x|\mu_i, \Sigma_i) = \frac{1}{(2\pi)^{n/2}|\Sigma_i|^{1/2}} \exp \left( -\frac{1}{2} (x - \mu_i)^\top \Sigma_i^{-1} (x - \mu_i) \right) \quad (8.6) $$

with $\mu_i$ mean and $\Sigma_i$ covariance. The EM algorithm iteratively calculates the parameters, $\lambda$, that maximize the likelihood function. It does this by first taking parameter estimates at iteration $k$ ($\lambda^k$) and calculating the expected value of the log likelihood function (the E-step). Then, the M-step calculates $\lambda^{k+1}$ values that maximize the log likelihood function from the previous E-step. Ref. [74] demonstrates that MLE estimates of $\lambda$ can use a “special case of the expectation-maximization (EM) algorithm” [70].

The GMM calculates data-cluster identities (DCIs) for the WT data (probabilistically identifies which data belongs with each cluster). The GMM DCIs for the slat $C_p$ data at wing tip port 133 in Figs. 8.2a and 8.2b are shown as colored dots in Fig. 8.3. There are two DCI calculations demonstrated in this plot, which is true for every pressure port on the slat, spar and flap; one set of calculations for flow near 0° and another set for flow near 36°. The black and blue dots indicate data belonging to separated and attached data clusters, respectively, near the 0° flow separation
location, and the red and blue dots represent data belonging to separated and attached data clusters, respectively, near the 36° flow separation location. The author learned that the GMM algorithm’s ability to determine which data points belonged to attached and separated flow regions depended on which data points were included in the GMM algorithm calculations. For example, if data points above $\alpha \approx 5^\circ$ were included in the GMM DCI calculations for flow near $0^\circ$, then the algorithm would sometimes erroneously assign data points below $0^\circ$ to the same data cluster as data points near $\alpha = 7^\circ$ and $10^\circ$. Therefore, the GMM DCI calculations for the flow separation regions near $\alpha = 0^\circ$ and $36^\circ$ only included data on the intervals $\alpha = [-4^\circ, 5^\circ]$ and $[30^\circ, 38^\circ]$, respectively. The GMM algorithm did not need the data in between the flow separation regions ($\alpha = [5^\circ, 30^\circ]$) to calculate the DCIs—these “unused data” points in the GMM algorithm (they are used in the overall process of building the $C_p$ surrogate as a function of $\alpha$) are illustrated as green dots in Fig. 8.3. Despite using the data subsets as inputs to the GMM algorithm, it did not always perfectly calculate the DCIs. For example, the DCIs in Fig. 8.3 near $0^\circ$ for slat port 133 at the wing tip show that the GMM algorithm incorrectly identified the pressure data point just above $0^\circ$ ($\alpha = 0.51^\circ$) as being part of the separated data (signified by the black dot), even though it appears to be part of the attached-flow data (the rest of
which is identified with blue dots) because of the small change in $C_p$ relative to the attached flow. Perhaps the GMM algorithm makes the argument that the change in $C_p$ slope between the data point at $\alpha = 0.51^\circ$ and the next data point indicates that the data point at $\alpha = 0.51^\circ$ should belong with the rest of the separated-flow data. By and large, the GMM algorithm did calculate the DCIs correctly for all pressure ports of the slat, spar, and flap, but there were some erroneous results at the 0° flow separation region, just as in Fig. 8.3 (there were no errors near 36°). In the effort to create a more automated surrogate modeling process of $C_p$ as a function of angle of attack for the WT data, a few port-location GMM DCI errors may be acceptable.

In summary, the Gaussian mixture modeling helped divide the data into subsets for the attached and separated flow regions in preparation to build the surrogate models described in Sections 8.1.5 and 8.1.6. Employing the GMM algorithm enables a more automated process in building the $C_p(\alpha)$ surrogate models.

8.1.5 Product of Experts

The product-of-experts (PoE) approach builds Gaussian process models to subsets of the data (for this application, the subsets are points identified as having separated flow and attached flow), and then combines each model representing the subsets together to form a single PoE model. Each GP model to a subset of the data is called an “expert.” The equations for this section and Section 8.1.6 come from Ref. [69], and the nomenclature is adapted for the angle of attack predictions in Section 8.1.3. The PoE predictive equation for the actual process, $f_\star$, at test locations, $x_\star$, is

$$p(f_\star|x_\star, D) = \prod_{i=1}^{M} p_i \left( f_\star | x_\star, D^{(i)} \right)$$  \hspace{1cm} (8.7)$$

where each of the $M$ experts ($M$ GP models) generates predictions for the entire data set $D$, and not just predictions at their respective subset data locations, $D_s$. Figure 8.4 provides a simple illustration of Eq. (8.7) in combining the distributed GP model computations together into a single PoE-predictive model. Equation (8.7) demonstrates that each of the GP experts in the PoE approach hold “veto” power,
in that if one expert assigns low probability to data values, \( p_i(f_*|x_*, D^{(i)}) \), then the resulting PoE probability is low [22].

\[
\mu_{\text{poe}}^{\mu}, \sigma_{\text{poe}}^{\sigma} \\
\mu_1, \sigma_1 \quad \mu_2, \sigma_2 \quad \mu_3, \sigma_3 \quad \mu_4, \sigma_4 \quad \mu_M, \sigma_M
\]

Figure 8.4.: Hierarchical 1-layer PoE model.

Combining the Gaussian predictions together results in a Gaussian with the respective mean and precision (inverse of variance) predictive equations

\[
\mu_{\text{poe}}^{\mu} = \left(\sigma_0^{\text{poe}}\right)^2 \sum_{i=1}^{M} \sigma_i^{-2}(x_*) \mu_i(x_*)
\]

\[
(\sigma_0^{\text{poe}})^{-2} = \sum_{i=1}^{M} \sigma_i^{-2}(x_*).
\]

Notice that GP experts that express much higher confidence (higher precision, or lower variance) in a data point’s value tend to overwhelm the experts with low confidence. Therefore, if one of the lower-level GP models erroneously expresses too much confidence in a prediction, the final PoE prediction will be skewed [22]. This excessive confidence could happen, for example, if the GMM algorithm incorrectly predicts that a data point from the attached flow region belongs to the separated flow data, and then the GP model for the separated flow would have to account for the attached-flow data point creating bias in the GP mean prediction and undue confidence in this specific GP model at the attached-flow data point. This over-confidence could also occur if the GP model variance hyperparameter estimates are lower than they should be for the given data.
8.1.6 Generalized Product of Experts

The generalized product of experts (gPoE) is an extension of the PoE approach which allows the user to input confidence, or belief, in each lower-level GP model’s (i.e., expert’s) predictions. This input is in the form of belief weights applied to each GP expert. These belief weights are similar to those in Section 7.2 in that they must sum to unity, \( \sum_i w_i = 1 \), can vary with the independent variable values (here, \( \alpha \) instead of \( s \) and \( \eta \) in Section 7.2), and combine multiple models together. However, this gPoE approach allows \( C^0 \) discontinuities in the belief weights, e.g., a single GP expert’s belief weight can jump from 0.8 to 0.1, or vice versa. The PoE equations in Eqs. (8.7), and (8.8) change to (with the belief weights, \( w_i \))

\[
p(f_*|x_*, D) = \prod_{i=1}^{M} p_i^{w_i}(f_*|x_*, D^{(i)}) \tag{8.9}
\]

\[
\mu^\text{poe}_{*} = (\sigma^\text{poe}_{*})^2 \sum_{i=1}^{M} w_i(x_*)\sigma^{-2}_i(x_*)\mu_i(x_*) \tag{8.10}
\]

Thus, the user can specify the level of belief, or confidence, in each GP expert model both within and outside each expert’s domain subset, \( D^{(i)} \). Note that the belief weight, or confidence, is not a statistical confidence interval. The belief weights for each expert were set to 0.90 for data within its specific subset used to train the GP model, \( D^{(i)} \), and 0.05 for the rest of the data domain, \( D^{(-i)} \) (there are three experts, so two experts have a belief weight of 0.05 in the domain of the other expert’s training data).

8.2 Modeling Results

This section discusses and compares three approaches to model the pressure data as a function of angle of attack, \( C_p(\alpha) \), at a few example pressure ports. The comparisons are applicable across all ports on the slat, spar, and flap. These modeling
methods, in order of computational cost and setup difficulty, are: 1. generating one GP surrogate model for the entire angle of attack (AoA) domain (i.e., not using the product-of-experts (PoE) approach); 2. combining multiple GP experts in a PoE approach; and 3. incorporating user belief weights on multiple GP experts with the generalized product-of-experts (gPoE) approach.

8.2.1 Single Gaussian Process

The results here are for the single GP model expert, i.e., using the entire pressure data set over angle of attack to train just one GP model.

The GP mean predictions in Fig. 8.5 for selected pressure port locations on different elements of the Trap Wing all smooth through the data in regions where the $C_p$ value seems to fluctuate with changing $\alpha$, but these predictions do not necessarily capture the onset of flow separation at the correct angle of attack. Figures 8.5b, 8.5d, and 8.5e illustrate that the GP models predict flow separation, but tend to represent the angle of attack at which flow separation occurs slightly after the actual flow-separation angle that the WT data indicates. That being said, all GP models in Fig. 8.5 do represent the data reasonably well. However, the uncertainty bounds on the prediction, reflected in the dashed lines that add or subtract the variance prediction to the mean prediction, seem excessive. The author investigated using tighter bounds on the values of the hyperparameters when solving the maximum likelihood estimation (MLE) problem to reduce the variance on the mean prediction, but this only resulted in numerical instabilities when the bounds were too restrictive. Therefore, the author kept wider bounds on the upper and lower values of the hyperparameters for the MLE.

8.2.2 Product of Expert and Generalized Product of Expert Results

The results in this section demonstrate the product of experts (PoE) and generalized product of experts (gPoE) models.
(a) Slat inboard ($\eta = 0.17$) port No. 4
(b) Slat wing tip ($\eta = 0.98$) port No. 133
(c) Spar inboard ($\eta = 0.17$) port No. 4
(d) Spar midwing ($\eta = 0.65$) port No. 133
(e) Flap midwing ($\eta = 0.41$) port No. 64
(f) Flap near wing tip ($\eta = 0.85$) port No. 161

Figure 8.5.: Single GP models of the Trap Wing $C_p(\alpha)$ values.
Figure 8.6 demonstrates the GP model prediction results for each expert, and the combined PoE and gPoE predictions. These results are from slat port number 133 at the wing tip—the same port data as in Figs. 8.2 and 8.3. The predictions

![Graphs showing coefficient of pressure vs angle of attack for different experts](image)

Figure 8.6.: GP model experts for Slat port No. 133 at $\eta = 0.98$.

for GP experts 1 and 3 in Figs. 8.6a and 8.6c were built to represent the points for separated flow at and below $\alpha = 0^\circ$ (GP expert 1) and for separated flow near and above $\alpha = 36^\circ$. At data subsets outside the training data, $D^{(-i)}$, these GP model predictions tend to follow the trend developed from representing the data in their respective training data subsets, $D^{(i)}$. And, as expected, the predicted uncertainties
associated with these individual expert GP models become very large far from the training data subset. The combined PoE and gPoE surrogate models in Fig. 8.7 show that the gPoE model represents the data better than the PoE model in general terms; the predicted value indicated by the solid black line lies much closer to the measured data.

Figure 8.7.: GP model experts combined into PoE and gPoE predictions for Slat port No. 133 at $\eta = 0.98$.

Figures 8.8a and 8.8b are close-up views of the flow separation regions in Fig. 8.7; these include the single GP model built to represent the entire data set, and these curves have no uncertainty predictions for viewing clarity. For this pressure port, the single GP model does a better job of representing the flow separation near zero degrees. This is somewhat expected because the GMM clustering algorithm incorrectly identified the data point at $\alpha = 0.51^\circ$ as a separated-flow data point (see Fig. 8.3). Because of this clustering error, the predictions of GP expert No. 1 (Fig. 8.6a) are skewed somewhat, so that the resulting PoE and gPoE are slightly skewed as well. This emphasizes the importance of correctly identifying the cluster to which the data belongs; the GMM clustering may not be suitable to “hands-off” automation for data at $\alpha = 0^\circ$. 
Figure 8.8.: Close-up views of separation regions for PoE, gPoE, and single GP models for Slat port No. 133 at \( \eta = 0.98 \). gPoE belief weights allow it to capture large \( C_p \) fluctuations.

The gPoE model does a better job than the PoE and single GP models of representing the data near the flow separation region close to \( \alpha = 36^\circ \) because it approximates the data more closely. The gPoE model approximates the data just before separation better because it combines multiple models together with belief weights that allow the mean prediction to get closer to the actual data point values before rapidly rising to capture the lower magnitude negative \( C_p \) values—an artifact of combining multiple GP experts with high belief weights at the data points they used to train their respective GP models. It also approximates the data after and during flow separation fluctuations near \( \alpha = 36^\circ \) better because combining weighted GP experts allows it to jump up to lower magnitude negative \( C_p \), indicating separation at this \( \alpha \), then back down to a higher magnitude negative \( C_p \) where the flow appears to be reattached at this \( \alpha \), and finally back up to capture the rest of the WT-measured flow-separated data. The green circles in Figs. 8.6, 8.7, and 8.8 are WT measurements. If the eventual merging process wanted to capture the oscillations in attached and separated flow near 36°, then the gPoE approach is the only method that the author investigated.
that is able to do this (researched single GP, PoE, cubic B-splines, and singular value decomposition (SVD) surrogate models). If the user does not want to interpolate the oscillatory data but would rather smooth through the oscillations, then the single GP model would be better than the PoE or gPoE models. This might be the case if the user recognizes that the flow separation / re-attachment / separation as $\alpha$ increases is potentially a transitory phenomenon due to unsteady, time varying flow, and the user would like the merging process to capture a single transition to separated flow. In terms of predicting the value of $\alpha$ where the pressure jump associated with separation occurs and predicting $C_p$ values above and below the separated flow / attached flow $\alpha$, the gPoE does the best of the three approaches investigated here, followed in order by the single GP model and the PoE model.

The gPoE seems to interpolate through the flow separation data that oscillates between $C_p$ values associated with separated and attached flow in Fig. 8.8b, but in reality the oscillations come from combining multiple GP experts that represent the measurement response from overlapping data domain subsets. The gPoE’s mean prediction, as a combination of the mean predictions and uncertainties from the three GP expert models in Fig. 8.6, captures the change in $C_p$ at the first instance of separated flow at $\alpha = 36.12^\circ$, the apparent reattachment at $\alpha = 36.16^\circ$, and then the separation again at $\alpha = 36.37^\circ$. As mentioned in Section 8.1.6, the author assigned belief weights of 0.90 for each GP expert model’s predictions at training data locations for that model, and 0.05 outside the training data set locations. The last data point GP expert No. 2 uses as training data in Fig. 8.6b is at $\alpha = 36.16^\circ$, and the first and second data points GP expert No. 3 uses as training data in Fig. 8.6c is at $\alpha = 36.12^\circ$ and 36.37°. So, the gPoE captures the rise and fall of the $C_p$ with uncertain flow separation locations by combining all three GP expert models with 90% belief weights in the predictions at the training locations and 5% everywhere else.

Figure 8.9 plots the PoE and gPoE results for the same wing elements and ports as the single GP models in Fig. 8.5. The uncertainties on the PoE and gPoE model mean predictions are generally smaller in the flow separation regions compared with
Figure 8.9.: PoE and gPoE GP models of the Trap Wing $Cp(\alpha)$ values.
the single GP model’s prediction uncertainties because the GP expert models in the flow separation regions had lower variance in those flow separation regions leading to lower variance in the combined PoE or gPoE models (Examine Eqs. (8.8) and (8.10) to understand how low variance in one GP expert model leads to low PoE and gPoE predictive variance.). However, the PoE and gPoE uncertainties on the mean predictions are about the same in the attached-flow regions compared with the single GP model uncertainties. This is because more data points in the attached-flow region led to higher variance from the GP expert hyperparameter estimates. Qualitatively, the gPoE seemed to model the data and locations of flow separation better than the single GP or PoE models. For instance, in Fig. 8.9b—which is likely one of the most difficult / problematic locations to predict and measure flow—the black line is closer to the green circles than the red line is. The flow separation region at \( \alpha \approx 36^\circ \) is fairly obvious in Figs. 8.9a, 8.9b, 8.9d, 8.9e, and 8.9f. The \( \alpha \approx 0^\circ \) flow separation region is most evident in Figs. 8.9b and 8.9f.

The gPoE appeared to better represent the wind tunnel data, but the computational cost to construct this model is higher than the single GP model. Table 8.1 lists the computational cost to build the single GP model and all of the GP model experts for the PoE model approaches (PoE and gPoE models have the same cost, because they involve the same steps to find the hyperparameters). The required time

<table>
<thead>
<tr>
<th></th>
<th>Single GP</th>
<th>PoE / gPoE</th>
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<tbody>
<tr>
<td></td>
<td>Mean (sec)</td>
<td>Std. (sec)</td>
</tr>
<tr>
<td>Slat</td>
<td>24.3</td>
<td>2.7</td>
</tr>
<tr>
<td>Spar</td>
<td>24.3</td>
<td>2.5</td>
</tr>
<tr>
<td>Flap</td>
<td>24.3</td>
<td>2.7</td>
</tr>
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Table 8.1: Computational cost of modeling \( \hat{C}_p(\alpha) \) at each pressure port

to build the models is very consistent across the three different wing elements because all pressure ports measured \( C_p \) at all \( \alpha \) in the wind tunnel test. The PoE / gPoE
approach costs 2.9 times more than the single GP model approach which also seems to make sense, because the POE and gPoE both need three individual GP “experts”. So, the trade-offs in accuracy and computational cost will influence whether a user should use a gPoE or a single GP model approach to represent pressure port data as a function of angle of attack.

8.2.3 Error Assessment

This section compares and discusses the error associated with the single GP, PoE, and gPoE methods of modeling the pressure data as a function of angle of attack.

Figure 8.10 shows RMSE as a function of angle of attack for the slat, spar, and flap wing elements; the inset plots use a different scale to focus on the values of $\alpha$ around the 36° separation location. While the error metrics correspond to discrete pressure port locations, the line plot used here better illustrates the trends. The error equations in Table 2.1 use $n$ equal to the number of pressure ports for each respective wing element. The highest error values clearly align with the flow separation points—near 0° and 36° angles of attack. Overall, the gPoE approach generated surrogate models with the lowest error, but there are a few angles of attack at which the single GP modeling approach generated lower error.

Figure 8.11 presents the standard error of the mean (SEM) value for each pressure port; this appears as a line plot as if SEM was a function of pressure port number to illustrate the trend better than a symbol plot. The SEM trend in Fig. 8.11 reinforces the conclusion from Fig. 8.10 that the gPoE approach produces surrogates with lower error compared with the single GP and PoE approaches. In several port locations, where the SEM value increases, the gPoE value of SEM is notably lower than that of the single GP and the PoE. The peaks and valleys in error values in Fig. 8.11 result from the port numbering. The pressure port numbering starts at the inboard pressure port band ($\eta = 0.17$) at the lower surface trailing edge, wraps around the leading edge, and then ends at the upper surface trailing edge before moving to the next outer band.
Figure 8.10.: GP model RMSE for the a) slat, b) spar, and c) flap summed over all ports for each angle of attack.

The last band is near the wing tip ($\eta = 0.98$). Thus, higher and lower SE values are associated generally with ports near the leading and trailing edges, respectively, as shown in Fig. 8.12 for the spar. This trend is also evident in results for the slat and flap shown in Fig. D.7 of Appendix D. Figure 8.12 shows modest SEM error values on the lower surface from the trailing edge toward the leading edge ($s = [0, 0.35]$), but the SEM error metrics rise substantially near the leading edge before dropping off dramatically toward the upper surface trailing edge ($s = [0.7, 1.0]$). The flap has
Figure 8.11.: GP model SEM for the a) slat, b) spar, and c) flap summed over all angles of attack for each pressure port.

Flow impinging on it from the upstream slat and spar wing tip vortices, which could be causing increasing unsteadiness leading to increased modeling error.

The purpose of building the wind tunnel $C_p$ surrogate model as a function of angle of attack, $\hat{C}_{p,WT}(\alpha)$, was to make a step towards developing a methodology to combine WT data and CFD results into a single merged $\hat{C}_{p,merged}(s, \eta, \alpha)$. The next step after building the wind tunnel $C_p$ surrogate model as a function of angle of attack, $\hat{C}_{p,WT}(\alpha)$, with either the single GP model or the gPoE is to generate the
Figure 8.12.: GP model SEM as a function of arc length for the spar summed over all angles of attack.

CFD surrogate as a function of angle of attack, $\tilde{C}_{p,CFD}(\alpha)$. One possible method to do this would be to use the WT surrogate $\tilde{C}_{p,WT}(\alpha)$ as the model basis function in Section 4.2 to build a GP model of the CFD results. Then, combine the surrogates in $s$ and $\eta$ with the $\alpha$ surrogates to form $\tilde{C}_{p,WT}(s, \eta, \alpha)$ and $\tilde{C}_{p,CFD}(s, \eta, \alpha)$, which are then merged to form the single merged $\tilde{C}_{p,merged}(s, \eta, \alpha)$. 
9. DISCUSSION AND CONCLUSION

The motivation behind this dissertation was to investigate methods to merge $C_p$ data from experimental WT data and CFD simulation results for use in several potential applications. While aerodynamicists and other aerospace engineers regularly perform some level of merging $C_p$ data from both sources, the specific efforts of this dissertation were seeking a method that would be more automated or “hands-off” and that would follow a more structured, perhaps less ad hoc, approach than current practice. A large part of the motivation for developing the merging process was to also provide a method to predict the best possible $C_p$ as a function of wing location and flow condition. Using the Trap Wing as a relevant example of a transonic wing with a multi-element high-lift system and available wind tunnel data and CFD results from the First AIAA CFD High Lift Prediction Workshop, this meant the ultimate goal was to have a merged $\hat{C}_p(s, \eta, \alpha)$.

This chapter discusses suggestions for future related work, and summarizes the results of this dissertation.

9.1 Future Work

Additional work could conduct more studies on the possibility of modeling pressure as a function of wing geometry and angle of attack simultaneously. Research efforts to this point indicate it is not feasible with the available data from the NASA Trap Wing CFD results and wind tunnel studies, but it would be beneficial for engineers if it were possible. The next steps to developing a merged $C_p(s, \eta, \alpha)$ would be to investigate building CFD $C_p(\alpha)$ surrogates with GP models using the WT surrogate $\hat{C}_{p,WT}(\alpha)$ as a model basis function. Then, research methods of combining $C_p(\alpha)$ and $C_p(s, \eta)$ surrogates into a single $C_p(s, \eta, \alpha)$ surrogate.
A natural extension of this work is determining pressure port placement on a wind tunnel model to maximize information gain from a wind tunnel experiment, because the merged $C_p$ distribution should inform the engineer of wing surface locations that need more WT measurements. For example, obtaining WT data from the slat lower surface trailing edge for the surrogates in Fig. 4.1 could be very helpful to generating more accurate $C_p$ surrogates, and in determining the surrogates’ predictive accuracy. The merged data set from this work can be used in a design of experiments calculation to maximize information gain, or mutual information (minimize uncertainty in predictions) [36,75]. A pressure port placement design of experiments that maximizes information gain would add ports to wing surface locations that minimize the uncertainty predictions of a GP model built using the merged $C_p$ distribution as “training data.” The algorithm could stop adding ports once a threshold in information gain is reached. Optimizing the pressure port placement could greatly increase the information gained from expensive wind tunnel experiments and help engineers better understand the various regions of the design space.

9.2 Summary of Contributions

This dissertation investigated methods and approaches to combine computational and experimental aerodynamic pressure data to not only increase information accuracy and quantity for aircraft designers, but to also decrease design cost. This work expands on the efforts of others that developed surrogate modeling tools (cubic B-spline, multi-fidelity, and Gaussian process) by building surrogate models of fields of pressure data to allow the merging process to predict $C_p$ at any location on the wing. Subject matter experts at Boeing suggested that modeling the CFD $C_p$ distribution may be a difficult, but this work demonstrates that the two-dimensional (2-D) cubic B-spline built using dyadic knot addition provides a highly credible surrogate model of the CFD $C_p$ distribution as a function of arc length and span. This work investigated combining 1-D GP models in one independent variable with the multi-fidelity concept
of additive corrector values. This additive corrector approach was computationally efficient, but not sufficiently accurate, as investigated here, to be an effective surrogate modeling approach for the WT $C_p$ data. Building an acceptably accurate surrogate model of the $C_p$ distribution on the wing surface—particularly from the wind tunnel data—was incredibly challenging. However, this work demonstrated that the use of Gaussian processes (GPs), particularly with the CFD B-spline surrogate as a model basis function, provided a generally acceptable surrogate model of $\hat{C}_p(s, \eta)$ to represent the wind tunnel data. Qualitative and quantitative comparisons of sequential and batch GP models demonstrate that the batch GP is the slightly better surrogate modeling approach (see Table 6.3). This dissertation effort investigated two merging approaches of the CFD and WT $C_p$ surrogates: 1) using the GP model, and 2) via user-defined belief weights. Generating a single, combined $C_p$ data set from WT and CFD data in a completely automated manner is extremely difficult, and may be impossible, without some amount of engineer supervision. This work demonstrated opportunities for automation of portions of the merging process.

Additionally, this research effort presented an initial effort to represent aerodynamic pressure data as a function of angle of attack, while accounting for and modeling discontinuous data in the form of flow separation.

### 9.3 Summary of Merging and Modeling Methods

Surrogate models represent the data sources for both computational fluid dynamic (CFD) simulation results and measured wind tunnel (WT) data in the merging process. Cubic B-splines surrogates approximate CFD simulation $C_p$ results. All wind tunnel (WT) surrogates used the CFD B-spline surrogate as a model basis function to improve modeling away from the WT data locations; this is an important aspect of building credible surrogates for the wind tunnel $C_p$ distribution over the surface of the wing elements. The WT surrogate methods employed and compared an additive corrector approach that borrowed concepts from multi-fidelity analysis used in multi-
disciplinary design optimization, sequential GP (two 1-D GPs in series), and batch GP (2-D GP parameters computed all at once) surrogates for modeling wind tunnel (WT) pressure data. To the author’s knowledge, no other published work investigates these approaches to modeling $C_p$ as a function of wing surface location. A full factorial design of experiments sampled the 2-D batch GP to evaluate which covariance functions are most significant in modeling the WT pressure data. Results indicate that the neural network, squared exponential, and Matérn covariance functions are most effective in the arc length direction, and none of the covariance functions in span ($\eta$) appeared to significantly improve the GP modeling accuracy.

Qualitative and quantitative comparisons were made between the three different methods. The qualitative assessment indicated that the sequential GP approach approximates the data at the data locations well, but the batch GP better approximates the flow physics away from data locations. This ability to represent the $C_p$ data at measurement locations and predict away from measurements is key for engineers, which is one reason why the author believes the batch GP to be a better surrogate over the sequential GP for the WT $C_p$ data. Also, the batch GP can handle data that is not necessarily in a grid format, while the sequential GP and additive corrector need $C_p$ data that is parallel to the arc length direction. The quantitative assessment indicated that the sequential GP generally had lower residuals than the other two methods, but much higher computational cost. The batch GP seemed to provide the best compromise of computational cost and surrogate modeling accuracy of the methods evaluated in this work.

The efforts here also recognized different perspectives on merging computational and experimental aerodynamic pressure data surrogates. One perspective is that using the CFD B-spline surrogate as a model basis function in construction of the WT GP models is a type of “merging,” and the other perspective is that these are surrogates of the respective data sets and truly merging the data requires an additional step.
All versions of the WT data surrogates use the B-spline surrogate of the CFD results as a model basis function, which could serve as a “merging” because the resulting prediction uses information from both sources. In the GP approach, this model basis function concept seems to place more weight or importance on the \( C_p \) values from the WT, because the likelihood optimization seeks hyperparameter values that would allow the best possible prediction of the WT values at \( s, \eta \) locations where WT data is available. The shape of the CFD B-spline merely provides a “starting point” for the Gaussian Process approximation. In a different approach to the 2-D surrogate of the wind tunnel \( C_p \) data, the computationally inexpensive additive corrector method uses the CFD B-spline surrogate to define the shape of the spanwise distribution of the \( C_p \) while minimizing prediction error at all spanwise locations for a given arc length position; this, too, combines information from both sources to make a prediction of the 2-D WT-based \( C_p \) distribution, but the additive corrector approach gives more weight to the shape of the CFD prediction than to the \( C_p \) values of the WT data.

The weighted-sum approach to merging was also presented. In this approach, engineers place belief weights on each data source’s surrogate indicating the engineers’ belief as to which surrogate is closest to modeling the “true” \( C_p \) distribution. Whether the user implements the merging perspective of the GP model or the weighted-sum approach, the goal is to generate a pressure data set that provides information to the engineer that improves aircraft design and analysis in some way. This approach moves further away from the notion of a hands-off merging process, but appears to provide some desirable results. Because of the potential to obtain preferred results from the \( C_p \) prediction, this latter method might suggest that the “best” merging process might require additional user interaction.

Based on initial efforts to incorporate flow conditions as independent variables in the merging process, modeling the pressure as a function of angle of attack employed two main methods: a product-of-experts (PoE) approach, and using a single GP model. Within the PoE approach, two methods provided \( C_p \) predictions: the
PoE method; and the generalized PoE (gPoE), which used belief weights to indicate perceived accuracy of each expert in various domain locations. This work employed Gaussian mixture modeling to separate attached and separated flow regions and then generated surrogates using a product of experts approach to combine the models.

Most of the surrogate modeling methods required some level of empiricism on the author’s part in the form of experience from some trial and error efforts. This empiricism involved building CFD B-spline models by adjusting the termination criteria for the knot-adding algorithm in each dimension. This involvement in tuning the B-spline to meet a specific error threshold appears to evade easy automation or coding, because the computational cost of generating B-splines is low, and the user will need to qualitatively and quantitatively assess the CFD surrogate’s accuracy and adjust the termination criteria to meet the user’s desired approximation error threshold.

Based on the author’s experience, determining this error threshold a priori for general application of the $C_p$ merging approach is likely difficult, if not impossible. The approach to calculating additive corrector values did not require empiricism and can be automated—once again, acknowledging the assumption that the model basis function (here, CFD pressure data) represents the physics correctly in the dimension for which the additive corrector values are being calculated. As demonstrated previously in the document, using a corrector value that is constant with respect to spanwise position for each arc length location might be insufficient to capture the flow physics reflected in the wind tunnel data. Conversely, from the viewpoint of automating the merging process, the GP modeling (either for wing geometry or angle of attack dimensions) will need the user to define the type of correction functions and which covariance functions to use. For aerodynamic pressure data applications, the author recommends using the cubic B-spline surrogate of the CFD results as the model basis function.
9.4 Conclusion

The cubic B-spline surrogate model adequately models the CFD pressure data in wing geometry, under guidance from the user. The additive corrector provides the most consistent computationally inexpensive option for modeling the WT pressure data in wing geometry, but with usually larger residual errors between the prediction and the measured $C_p$ value at locations where the measurements are available. The sequential GP approximates the data well at the data locations in wing geometry, but this approach does not represent the overall flow physics well and is the most computationally expensive. The batch GP seems to provide the best compromise of computational expense and pressure data predictive capabilities. Benefits to using surrogate models are the ability to generate $C_p$ data predictions at any location on the wing and the “hands-off” approach needed to generate the $C_p$ distribution (this probably means that fewer engineers are needed in the discussion of how to merge the two data sources). Limitations with surrogate models are the fact that none are perfect and that they all require some level of user interaction, or in other words, “Far better an approximate answer to the right question, ... than an exact answer to the wrong question” [1]. Implementation of the above approaches requires some knowledge of the underlying approaches to build the surrogates.

Based on the preliminary investigations of building $C_{p,WT}(\alpha)$, there appear to be some open issues depending upon the user’s need from this surrogate. If the user needs the least computationally expensive option that is adequate, then a single GP model is best because it approximates the data well and is the least expensive. If the user needs the best method at predicting flow separation location, then the investigations to this point indicate that the generalized product of experts approach would be best.
LIST OF REFERENCES
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APPENDICES
A. PSEUDOCODE

Pseudo-code for the multivariate B-spline model.
Algorithm 1 Tensor Product B-spline

**Build 1-D B-spline for** $N$ spanwise stations in $s$ direction to $C_p(s)$:

for $j := 1$ to $N$ do

Knot-adding algorithm:

$t \leftarrow u = 0.5$ Add knot to domain midpoint ($u = 0.5$ for $u \in [0, 1]$)
error $\leftarrow r(u) - C_{p,CFD}(u)$

while $\max(||error||) > \text{Max}_{\text{allowable}}(||error||)$ do

Add knot to dyadic interval with maximum error

$t \leftarrow [t_i (t_i = \max(||error||) + t_{i+1})/2]$
end while

$t_j \leftarrow t$
end for

$T \leftarrow \bigcup_{j=1}^N t_j$

for $j := 1$ to $N$ do

$r(u) = \sum_{i=0}^m P_i(u) B^k_i(u)$ using the set $T$
end for

**Build 1-D B-spline for** $M$ arc length stations—same as above, except in span direction to $P$ from previous build direction:

for $i := 1$ to $M$ do

$r(v) = \sum_{j=0}^p P_j(v) B^k_j(v)$

Perform knot-adding algorithm
end for

$T_{\text{span}} \leftarrow \bigcup_{i=1}^M t_i$

for $i := 1$ to $M$ do

$P_{i,j}(v) \leftarrow (B^k(v))^{-1} P_i(v)$
end for
B. COMPARING COVARIANCE KERNELS FOR 2-D WIND TUNNEL GAUSSIAN PROCESS MODELS

This appendix provides more information regarding the kernel comparison discussed in Section 4.3.2. In that section, Fig. 4.3 displays the main and interaction effects plots for the MAE metric of slat two-dimensional (2-D) wind tunnel (WT) Gaussian process (GP) at $\alpha = 6^\circ$. This section provides additional effects plots that demonstrate the relative importance of the kernel factors in the MAE error metric for each wing element at each angle of attack. The response metric for this full factorial design of experiments is the mean absolute error (MAE) of the residuals for all pressure ports from each wing element, $e_k = C_{p,WT}(x_k) - \hat{C}_{p,WT}(x_k)$

$$\text{MAE} = \frac{1}{n} \sum_{i=1}^{n} |e_i|.$$  \hspace{1cm} (B.1)

Figures B.1 and B.2 illustrate that the conclusions from the main effects plot in Fig. 4.3 is true for these two metrics as well.

Figures B.3 through B.28 are extensions of the main and interaction effects plots in Section 4.3.2. Each wing element (slat, spar, and flap) have main and interaction effects plots either in Section 4.3.2 or here for $\alpha = 6^\circ, 21^\circ, 32^\circ, 34^\circ, \text{and } 37^\circ$. 
Figure B.1.: Slat 2-D WT GP $L^2$-norm main effects for $\alpha = 6^\circ$.

Figure B.2.: Slat 2-D WT GP RMS main effects for $\alpha = 6^\circ$. 
Figure B.3.: Slat 2-D WT GP MAE main effects for $\alpha = 21^\circ$.

Figure B.4.: Slat 2-D WT GP MAE two-factor interaction effects for $\alpha = 21^\circ$. 
Figure B.5.: Slat 2-D WT GP MAE main effects for $\alpha = 32^\circ$.

Figure B.6.: Slat 2-D WT GP MAE two-factor interaction effects for $\alpha = 32^\circ$. 
Figure B.7.: Slat 2-D WT GP MAE main effects for $\alpha = 34^\circ$.

Figure B.8.: Slat 2-D WT GP MAE two-factor interaction effects for $\alpha = 34^\circ$. 
Figure B.9.: Slat 2-D WT GP MAE main effects for $\alpha = 37^\circ$.

Figure B.10.: Slat 2-D WT GP MAE two-factor interaction effects for $\alpha = 37^\circ$. 
Figure B.11.: Spar 2-D WT GP MAE main effects for $\alpha = 6^\circ$.

Figure B.12.: Spar 2-D WT GP MAE two-factor interaction effects for $\alpha = 6^\circ$. 
Figure B.13.: Spar 2-D WT GP MAE main effects for $\alpha = 21^\circ$.

Figure B.14.: Spar 2-D WT GP MAE two-factor interaction effects for $\alpha = 21^\circ$. 
Figure B.15.: Spar 2-D WT GP MAE main effects for $\alpha = 32^\circ$.

Figure B.16.: Spar 2-D WT GP MAE two-factor interaction effects for $\alpha = 32^\circ$. 
Figure B.17.: Spar 2-D WT GP MAE main effects for $\alpha = 34^\circ$.

Figure B.18.: Spar 2-D WT GP MAE two-factor interaction effects for $\alpha = 34^\circ$. 
Figure B.19.: Flap 2-D WT GP MAE main effects for $\alpha = 6^\circ$.

Figure B.20.: Flap 2-D WT GP MAE two-factor interaction effects for $\alpha = 6^\circ$. 
Figure B.21.: Flap 2-D WT GP MAE main effects for $\alpha = 21^\circ$.

Figure B.22.: Flap 2-D WT GP MAE two-factor interaction effects for $\alpha = 21^\circ$. 
Figure B.23.: Flap 2-D WT GP MAE main effects for $\alpha = 32^\circ$.

Figure B.24.: Flap 2-D WT GP MAE two-factor interaction effects for $\alpha = 32^\circ$. 
Figure B.25.: Flap 2-D WT GP MAE main effects for $\alpha = 34^\circ$.

Figure B.26.: Flap 2-D WT GP MAE two-factor interaction effects for $\alpha = 34^\circ$. 
Figure B.27.: Flap 2-D WT GP MAE main effects for $\alpha = 37^\circ$.

Figure B.28.: Flap 2-D WT GP MAE two-factor interaction effects for $\alpha = 37^\circ$. 
C. COMPARING 2-D WIND TUNNEL SURROGATE MODELS

This appendix chapter discusses and compares wind tunnel surrogate modeling results for $C_p(s, \eta)$.

C.1 Surrogate Surface Plots

This section demonstrates WT surrogate results for sequential GP, batch GP, and additive corrector using surface plots.

Section 4.4.3 discussed a few results of the 2-D sequential GP model. Of particular note are the ability to approximate the data, but with some wild extrapolations. Figures C.1 and C.2 show the spar $C_p$ at $\alpha = 6^\circ$ with some extraneous pressure spikes near the leading edge ($s \approx 0.5$) near the body pod and at the wing tip ($y/b = \eta = 0$ and 1, respectively).

Figures C.3, C.4, and C.5 demonstrate the batch GP method for the slat at the same flow condition ($\alpha = 37^\circ$) as the sequential method in Fig. 4.15. These results reinforce the idea above lessons learned from the flap surrogates that the batch GP surrogate: 1. does not approximate the WT data at the data points as well as the sequential method, 2. does generate more reasonable surrogate approximations away from the data points compared with the sequential method, and 3. hence, increasing the degrees of freedom for the batch surrogates should improve approximation accuracy at the data points.

Figures C.6, C.7, and C.8 display the flap 2-D WT additive corrector surrogates at $\alpha = 21^\circ$.

Figures C.9, C.10, and C.11 display the spar 2-D WT additive corrector surrogates at $\alpha = 6^\circ$. 
Figure C.1.: Spar 2-D sequential GP surrogate at $\alpha = 6^\circ$.

Figure C.2.: Additional views of spar 2-D sequential GP surrogate at $\alpha = 6^\circ$.

**C.2 Residuals and Error Metrics**

This section shows additional residual and error metric plots for the WT surrogate results from sequential GP, batch GP, and additive corrector surrogates.
Figure C.3.: Slat 2-D batch GP surrogate at $\alpha = 37^\circ$.

Figure C.4.: Additional views of slat 2-D batch GP surrogate at $\alpha = 21^\circ$.

The surrogate residuals in Fig. C.12 for the slat are averaged over all angles of attack. The slat residuals are larger near the leading edge ($s \approx 0.5$) and somewhat larger near the wing tip, as expected.
The residuals in Fig. C.13 demonstrate the same trend as the flap residuals in Figs. 6.1 and 6.2.

The boxplots of the absolute residuals in Figure C.14 illustrate the surrogate approximation errors at all pressure ports, outliers, and a relative absolute residual distribution. The slat boxplot in Fig. C.14a demonstrates that the additive corrector has larger absolute residual values, but not as large of outliers as the two GP methods. The sequential approach (labeled as Two 1-D GPs in the figures) generally has more error than the batch method (labeled as 2-D GP) for the slat at $\alpha = 36^\circ$. The boxplots in Fig. C.14 demonstrate a wide variety of absolute residual values across the different wing elements. Also, in looking at the top whisker among the three methods for the three wing elements shows that the additive corrector method generally has larger absolute residual values, but the sequential GP approach displays some inconsistency because it has larger errors on the spar than the others. In short, looking at just one
Figure C.6.: Flap 2-D WT additive corrector surrogate at $\alpha = 21^\circ$.

Figure C.7.: Profile views of the flap 2-D additive corrector surrogate at $\alpha = 21^\circ$.

wing element or one angle of attack is not sufficient to decide which surrogate is most appropriate for this Trap Wing example.
Figure C.8.: Opposing view of flap 2-D additive corrector surrogate at $\alpha = 21^\circ$.

The following ECDF plots illustrate additional surrogate error distributions beyond those in Chapter 6.
Figure C.9.: Spar 2-D WT additive corrector surrogate at $\alpha = 6^\circ$.

Figure C.10.: Profile views of the spar 2-D additive corrector surrogate at $\alpha = 6^\circ$. 

(a) $C_p$ vs. arc length
(b) $C_p$ vs. span
Figure C.11.: Opposing view of the spar 2-D additive corrector surrogate at $\alpha = 6^\circ$.

Figure C.12.: Mean slat surrogate residuals averaged over all angles of attack.
Figure C.13.: Mean spar surrogate residuals averaged over all angles of attack.

(a) Arc length

(b) Span
Figure C.14.: Absolute residual boxplots for each surrogate at $\alpha = 36^\circ$. 
Figure C.15.: Absolute residual ECDF for each surrogate at $\alpha = 13^\circ$. 
Figure C.16.: Absolute residual ECDF for each surrogate at $\alpha = 34^\circ$. 
Figure C.17.: Absolute residual ECDF for each surrogate at $\alpha = 36^\circ$. 

(a) Slat

(b) Spar

(c) Flap
D. MODELING ERROR OF PRESSURE DATA OVER ANGLE OF ATTACK

This section plots surrogate modeling error metrics of the pressure data as a function of angle of attack, \( C_p(\alpha) \). The surrogate models are: 1) a single GP model to the data, 2) a product-of-experts (PoE) model, and 3) a generalized product-of-experts (gPoE) model. The associated equations come from Table 2.1.

The first set of figures (Figs. D.1, D.2, and D.3) show the mean absolute error (MAE), \( L^\infty \)-norm, and standard error of the mean (SEM) metrics as a function of angle of attack summed over the \( n \) pressure ports. The second set of figures (Figs. D.4 D.5, and D.6) displays the root mean square error (RMSE), mean absolute error (MAE), and \( L^\infty \)-norm metrics as a function of the pressure port number on the wing summed over the \( n \) angles of attack.

Figure D.7 provides additional evidence of the higher SEM error near the leading edge (around \( s = 0.5 \)) as opposed to the lower and upper surface trailing edges (\( s = 0.0 \) and 1.0, respectively).
Figure D.1.: GP model MAE for the a) slat, b) spar, and c) flap summed over all pressure ports for each angle of attack.
Figure D.2.: GP model $L^\infty$-norm for the a) slat, b) spar, and c) flap summed over all pressure ports for each angle of attack.
Figure D.3.: GP model SEM for the a) slat, b) spar, and c) flap summed over all pressure ports for each angle of attack.
Figure D.4.: GP model RMSE for the a) slat, b) spar, and c) flap summed over all angles of attack for each pressure port.
Figure D.5.: GP model MAE for the a) slat, b) spar, and c) flap summed over all angles of attack for each pressure port.
Figure D.6.: GP model $L^\infty$-norm for the a) slat, b) spar, and c) flap summed over all angles of attack for each pressure port.
Figure D.7.: GP model SEM as a function of arc length for the slat and flap summed over all angles of attack.
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