Uncertainty Visualization Challenges in Decision Systems with Ensemble Data & Surrogate Models

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ABSTRACT

Uncertainty visualization is a key component in translating important insights from ensemble simulation data into actionable decision-making by visually conveying various aspects of uncertainty within a system. With the recent advent of fast surrogate models trained on ensemble data, we can substitute computationally expensive simulations, which allows users to interact with more aspects of data spaces than ever before. However, the use of ensemble data with surrogate models in a decision-making tool brings up new challenges for uncertainty visualization, namely how to reconcile and communicate the new and different types of uncertainties brought in by surrogates and how to utilize these new data estimates in actionable ways. In this work, we examine these issues as they relate to high-dimensional data visualization, the integration of discrete datasets and the continuous representations of those datasets, and the unique difficulties associated with systems that allow users to iterate between input and output spaces. We assess the role of uncertainty visualization in facilitating intuitive and actionable interaction with ensemble data and surrogate models, and highlight key challenges in this new frontier of computational simulation.

Index Terms: Ensemble data, surrogate models, uncertainty visualization

1 INTRODUCTION

Ensemble simulation is a popular approach for investigating ranges of possibilities, mitigating unknowns, or estimating error in complex computational systems [35]. By perturbing parameter settings and simulating numerous realizations, we can examine a broad view of possible dynamics, retrieve an understanding of parameter sensitivities, and determine confidence levels around system states. As ensemble simulations increase in complexity, visualization challenges are compounded. Specifically, the data are *multi-dimensional* as they consist of both spatial and temporal components. They are *multi-variable*, outputting tens to hundreds of variables. Finally, the ensemble data are *multi-valued* as they capture many realizations of the space-time-variable combinations. The size and complexity of ensemble data quickly overwhelm the limited number of visual channels in the design space and force visualization creators to make choices on how to reduce the data for communication. In the rest of this manuscript, we use the term *ensemble data* to refer to data produced from the actual computational simulation.

Simultaneously, novel artificial intelligence (AI) methods are rising in popularity, allowing us to train fast-running surrogate models that approximate simulations at a fraction of the computational cost. However, there exist trade offs in fidelity and uncertainty quantification, and nuances in what surrogates can estimate. This new capability allows us to query novel parameter settings and instantaneously retrieve predicted values and uncertainty estimations (as shown in Figure 1). These advances in AI and machine learning dramatically increase the simulation space users can explore, thus increasing the demand on the visual design space, and exacerbating visualization challenges.

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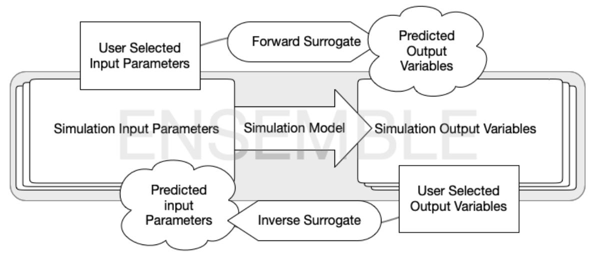

Figure 1: The relationship between ensemble datasets and surrogates. Parameters (left) and outputs (right) in solid rectangles represent realizations from an ensemble dataset. A forward surrogate (top) enables a user to propose novel parameter settings and predict output variables, along with quantified uncertainty relating to how close those predictions get to the original ensemble outputs. A reverse surrogate (bottom) allows the user to choose output values and determine possible input parameters that will get within a range of that proposed output.

Ultimately, comprehension of ensemble simulation paradigms combined with surrogate modeling is fundamental both for scientific inquiry and decision-making, as these systems gain wide traction across scientific domains. As surrogate models permeate computational modeling, such as in the use of digital twins, they become increasingly consequential to decisions that affect multiple aspects of daily life. Designing visualization systems that effectively convey ensembles and surrogate data, and the uncertainty contained within, remains an open, essential, and challenging area of research.

2 BACKGROUND AND RELATED WORK

A little over a decade ago, uncertainty visualization was called out as a critical next step for the visualization community [16]. Ensemble data are a unique formulation that enable exploration of uncertainty by simulating many runs of computational models. Due to their popularity [10, 34] the understanding of scientific simulation ensembles and their uncertainty have become central challenges in the visualization community [5, 23, 24]. Much research has been dedicated to exploring variability of simulation outputs, often relying on summary statistics and multi-window frameworks [25, 26, 35]. Visual parameter space exploration explicitly focuses on understanding the relationship between simulation inputs and simulation outputs [7, 27]. In each of these cases, the ability of a user to explore input-output relationships and build understanding of the dynamics of the system is constrained by the content of the ensemble itself. Not only are there computational challenges from running large-scale, complex systems with formidable data sizes, it is also unclear how to visually convey these data and their uncertainties in a manner that is appropriate for any particular decision maker [15] or address issues surrounding interpretation and usability of scientific data by non-experts [22].

Recently, fast surrogate models have helped address computational limitations and expand user flexibility in model exploration [1,4,9,13,18,30,31]. In scientific simulations, surrogates are typically machine learning-based models that can learn complex relationships from ensemble datasets, approximating the behavior of the original computational model. But, unlike an ensemble dataset composed of discrete simulation realizations, surrogates learn continuous representations of the input-output relationships. Consequently, a surrogate model enables a user to query an arbitrary set of input parameters, and immediately receive a predicted output as if they had just run the full simulation.

A particularly interesting and under-explored application of surrogate models in the visualization community is inverse analysis, which we define here as identifying a set of possible inputs from a specifically requested output. For clarity, we refer to surrogates that take inputs and produce outputs as *forward surrogates*. The process of going from output to inputs can be achieved through various methods, including intrinsically invertible surrogates [36], or through search algorithms [17]. Intrinsically invertible surrogates facilitate direct inversion, that is to say, outputs can be passed to the same model that did a forward inference, which then provides the corresponding inputs (or input distribution). Search algorithms, on the other hand, leverage the speed of forward surrogates to search through input space and evaluate predicted outputs for closeness to the requested output.

The type of surrogate model explicitly dictates the content and associated uncertainty of the model results. In principle, any mathematical model that sufficiently captures input-output relationships in the data could be used as a simulation surrogate. That being said, several categories of models have proven especially useful due to their instrinsic properties. Specifically, Gaussian processes (GPs) are probabilistic models that enable multivariate inputs and outputs, and inherently provide a quantification of uncertainty [20,28,32].

In cases of large-scale, multi-dimensional data (e.g., volumetric or geospatial), a deep learning model might more accurately capture small-scale details as well as global structure in the simulation output, where GPs tend to struggle. One such example is InSituNet [14], a generative, deep learning-based surrogate. In its original formulation, InSituNet learns the relationship between simulation parameters and completely composed 3D visualizations–images of a 3D reconstruction of the simulation outputs from a specified viewpoint. Conveniently, the overall architecture of InSituNet also allows it to learn a more straightforward matrix-style, 2D representation (i.e., image) of data resulting from a simulation.

However, unlike a GP, InSituNet does not intrinsically provide a quantification of uncertainty. In order to visualize uncertainty in its predictions, we would need to introduce additional methods, such as Monte Carlo dropout [12] or training multiple instances of the same model [6, 11, 19]. In general, uncertainty quantification and visualization of AI models is an area of active research [3, 13, 21, 29, 33]. Given that most surrogates are "black-box" models, understanding their stability and accuracy across input space is essential for trustworthiness and confidence in their results. High uncertainty in surrogate model predictions can occur because of insufficient data (i.e., not enough members in the ensemble used to train the surrogate) or imbalanced data distribution in certain regions (i.e., ensemble sampling fidelity is too high or irregular).

Although problems still exist in ensemble visualization and surrogate models for visualization, we argue here that unifying these sources is ultimately a fruitful endeavor in decision-making visualization systems. However, we also find multiple unique challenges with this integration, and identify opportunities for uncertainty visualization to help address them.

3 Flood Modeling Example

To illustrate important considerations for the visualization design of ensemble datasets combined with surrogate models, we explore modeling floods due to a dam breach, using the DSS-Wise Lite flood model [2]. At a high level, the flood model accounts for dam properties (e.g., materials, structure, reservoir characteristics), and detailed hydrology to capture water movement. The model computes variables describing a resulting flood including detailed spatial grids and aggregate geographic measures. We consider three main input parameters: breach width, breach failure elevation, and breach formation time and focus on the aggregate output variables of: maximum flood depth, maximum flood speed, the mean arrival time of the flood, and the number of people at risk due to the flood.

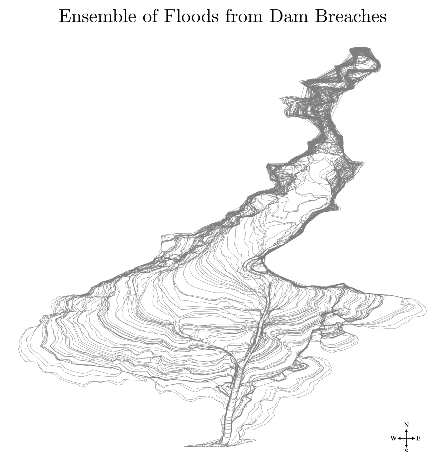

Figure 2: An ensemble visualization of the output variable *flood spread*. Each contour line represents a realization in the ensemble and the collective view shows the geographic range that the flood might reach.

3.1 Ensemble Data

Ensemble datasets are well-suited for describing global properties of parameter and outcome spaces. The primary goal of the flood model is to understand where a flood might occur and the level of damage that might be inflicted, particularly as it relates to populated areas. Figure 2 shows a contour of the flood spread for each member of the flood simulation. Specifically, we can see a range of contours that relate to how far down a valley a flood might reach. We show the ensemble of inputs and aggregate measures of the flood in the parallel coordinates plot of Figure 3, where each grey line indicates a member of the ensemble.

3.2 Surrogate Models

Surrogate models provide a means of exploring novel areas of simulation input and output space. In the context of the flood simulation, we may be interested in the flooding that would result from a dam break whose failure elevation and width are not represented in the original ensemble dataset. Or we might want to designate a particular distance of flood spread and use an inverse surrogate to provide potential input parameter settings. Such surrogates allow for a more refined interrogation of the model by enabling more localized queries in both the input and output space, thus facilitating multiple ways for a user to reason with the model.

For the flood data, we could choose a novel set of input parameters and get a prediction of output values using a Gaussian Process surrogate. The output prediction range of this forward surrogate is shown in Figure 3 by the blue shaded region. In a similar fashion, one could propose target values for the output space and use an inverse surrogate or search algorithm to then retrieve ranges of

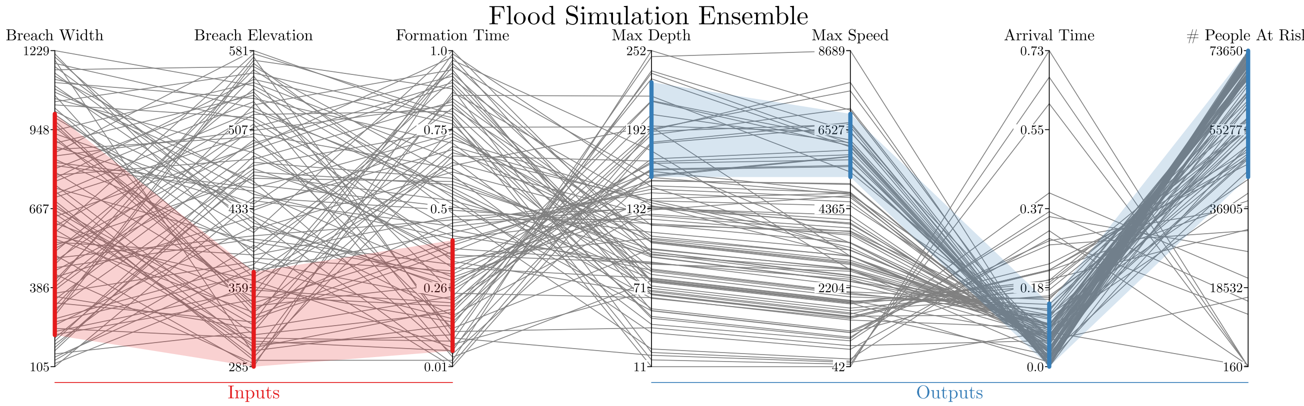

Figure 3: Parallel coordinate plot for a flood simulation ensemble. Input parameters are on the left hand side and output variables on the right. Grey lines represent individual ensemble realizations connecting specific values of input parameters and output variables. A forward surrogate prediction (predicting outputs using inputs) is shown as blue vertical lines for each output, with shading indicating the range of predicted output values. An inverse surrogate (predicting inputs using outputs) is shown as red vertical lines with the range of possible input parameters shaded in red.

input variables that might yield that request (such as the red shaded region in Figure 3). Figure 4 shows an example of a widget that could be used to specify the maximal depth of a flood. In this example, a user can move the red line to trigger an inverse surrogate model. This particular example limits the user to specifying values for a single output, but a more robust interface might allow for many outputs to be specified, but presents its own design challenge for a visualization system [8], which we discuss in more detail in the next section.

While the parallel coordinates plot in Figure 3 gives us a clear picture of the ensemble data and potential ranges of input or output values predicted from forward or inverse surrogates, it does not provide much, if any, insight of use in real-world decision-making. While we use the GPs to model relationships with scalar outputs, visualization surrogates like InSituNet could be used to model the entire flood-plane itself, including depth or speed values at each individual location, encoded as a geospatial heatmap. Figure 5 shows an example of a flood model visualization using InSituNet that gives greater context for the data. This sort of visualization is likely much more useful within a decision-making system. Understanding when and what types of surrogates to use in a particular sitation is a fundamental design challenge.

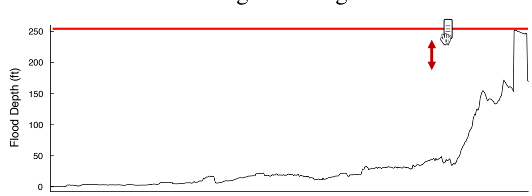

Figure 4: Example of a widget showing the flood depth profile. Users can move the red line to define a desired maximum flood depth which could then trigger a prediction from the inverse surrogate.

4 Visualization Challenges for Decision Making

Uncertainty visualization is a key component in addressing the challenges that arise from integrating ensemble data and surrogate models within a single visualization system. The interplay of the uncertainties associated with each of these sources is complex and important to consider when designing systems for supporting decision-making, particularly in critical situations such as flood modeling. Challenges inherent to ensemble visualization are exacerbated by the inclusion of surrogate modeling, and it is unlikely that any general approach will be appropriate for all situations.

Specifically, we have identified the following challenges that will need to be addressed in any system focused on visualizing uncertainty and integrating ensemble data with surrogate modeling:

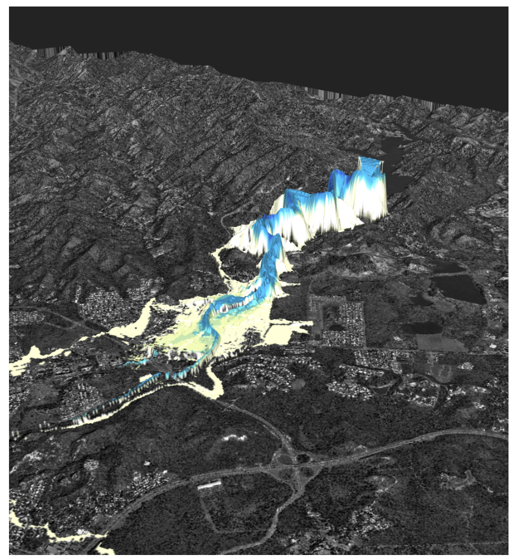

Figure 5: A visualization of the flood model generated using InSituNet. This image shows the height of the flood and is colored by highest hazard risk in blue (derived from max velocity).

1. Leveraging the strengths of ensemble data and surrogate models to contextualize and interact with global and local simulation space, while mitigating their respective limitations;
2. Clearly communicating the different types of uncertainties that arise from ensemble data and surrogate models;
3. Clarifying the complex relationships within and between inputs and outputs.

All of these challenges are relevant for assisting users in decision-making. In particular, each one is a crucial part in allowing users to obtain the correct information for a decision and accurately evaluate that information and their confidence in it.

4.1 Ensemble and Surrogate Model Interplay

Our first two listed challenges primarily address the complexities of using ensemble data and surrogate models together in visualization. Their synergies offer a strong argument for incorporating them both in a single visualization system, but there are a number of pitfalls that must be addressed.

Overall, the strength of ensemble data is in capturing global characteristics of simulation space, whereas surrogate models excel at facilitating local access to any point in that space. More concretely, ensemble data provide useful global information of parameter and output spaces, while surrogate models fill in gaps present in ensemble data, which can be important when analyzing local regions of simulation space. The complementary strengths of ensemble data and surrogate models is especially relevant in analyses that move between global and local investigations of simulation space.

As an example of our first listed challenge, consider the flood ensemble shown in the parallel coordinates plot of Figure 3, where the spread across each variable is immediately apparent by the layout of the grey lines across each coordinate. A task might be to identify partitions of arrival time that separates the number of people at risk into either tens of thousands vs. hundreds. We can see a large gap between ensemble members on the arrival time variable approximately between .37 and .55 hours, which has a clear relationship with the number of people at risk (longer arrival time leads to less people at risk). We could then use surrogate models to investigate that area in simulation space further to better determine at what arrival time the person's at risk variable increases significantly.

Although surrogate models are trained on ensemble data, they do not represent it perfectly. In regions of simulation space where surrogate prediction uncertainty is large, we may need to rely on ensemble data as a better representation of that space, or even discover the need to obtain more realizations of the original dataset and re-train our surrogates. In our flood simulation example, forward surrogate predictions for the outputs of the flood simulation are shown as blue shaded regions in Figure 3. The uncertainty associated with the prediction of the number of people at risk has a significant range, larger than twenty thousand people. In this case, it may make more sense to investigate the ensemble members directly to better understand what can cause such a drastic difference in people at risk.

However, the interaction between ensemble data and surrogate models must be handled with care. Poorly designed visualization systems could result in users iterating far too much between visualizations of ensemble data and surrogate predictions to try and understand discrepancies between them. Specifically, users need to know if differences between an ensemble member and a surrogate prediction are the result of the surrogate uncertainty (i.e., surrogate accuracy) or an actual change in the simulation space landscape (i.e., does the difference actually exist in the simulation space?). This highlights the importance of our second listed challenge.

4.2 Decision Making using Inputs and Outputs

A significant opportunity for decision-making visualization systems is the use of invertible surrogates—that is—models that can either take inputs and produce outputs or take outputs and produce inputs. This presents unique opportunities for visualization design, because we can facilitate interactions between inputs and outputs according to what makes the most sense to support a user's decision or their background knowledge. In our example flooding scenario, defining dam breaks (the inputs) may work for modelers or dam engineers deciding if the dam needs upgrades, because they have sufficient understanding of the relationship between dam breaks and hydrology. However, emergency planners deciding evacuation plans by assessing overall flooding risk likely benefit more from interaction with the *flood spread* (as in Figure 2) or the *number of people at risk* output measure.

While promising, there are challenges associated with surrogates that can go between inputs and outputs in either direction. Consider the case where a user queries a surrogate in one direction, and then uses that prediction to query the surrogate in the opposite direction, as in the red and blue shaded regions of Figure 3. Even with careful design of surrogates, poor communication of the uncertainty in the predictions could result in users drifting in simulation space in unintended ways. Designing interactions with surrogates that demonstrate to users how they are moving through simulation space, and why they end up in particular regions, is a crucial part of addressing challenges 2 and 3.

Moving within and between input and output spaces with surrogates is especially difficult for high-dimensional data where the relationships are more complex. Consider the case where a user defines an output and a surrogate returns possible sets of inputs that could produce that output (e.g., via a search algorithm that uses a forward surrogate). The dependencies between inputs is important information for users. Specifically, it is not enough for users to know the range of possible values for each input individually (as is currently shown in Figure 3), because the value of one input influences the possible values of the others. In the case of our flooding example, to see the same flooding for two different dam breaks with different elevations, the width and possibly the formation time must also be different. In other words, when a user requests a fixed output, it is not particularly useful to show the relationship between inputs and outputs. Instead, uncertainty visualizations must convey the *joint and conditional distributions* of inputs for a given output.

Lastly, although we can now design systems that allow users to define desired outputs and query for the inputs that produce them, it is not a guarantee that the request is a feasible realization according to the surrogate. This scenario must be treated with special consideration. It could mean the user does not understand a dependency between the requested outputs, and improved uncertainty visualization design that better conveys the relationship between the outputs could alleviate this issue. However, focusing solely on the relationship between the outputs misses a key opportunity to address an important analytical task in decision-making that is not well-addressed in the uncertainty visualization community. Specifically, this scenario highlights a natural way that trade-off analysis can arise within visualization systems, and warrants further exploration. When a user requests multiple outputs that are not achievable simultaneously, we can use uncertainty visualization to show the sets of inputs that result in the desired outputs individually, as well as sets of inputs that get as close to all desired outputs as possible (e.g., Pareto optimality). These kinds of complex trade-off analyses between multi-dimensional distributions of inputs and outputs are important for decision-making, and a unique opportunity for uncertainty visualization. Other analysis tasks relevant to decision-making may also arise as we learn more about the capabilities of surrogate models to facilitate interaction within and between input and output spaces.

5 Conclusion

In this work, we delineated three major challenges for visualization systems that incorporate both ensemble data and surrogate models, in the context of decision-making. Uncertainty visualization is a foundational component of such systems, as it influences users' understanding and reasoning with ensemble data and surrogate models, which impacts decision-making. We discussed the quickly evolving landscape of surrogate models, and the opportunities to utilize them in novel ways to support more intuitive decision-making within visualization systems. Furthermore, we highlighted how existing problems in ensemble and uncertainty visualization are exacerbated when incorporating ensemble data and surrogate models together. Namely, issues surrounding high-dimensional data, relationships, and uncertainties are compounded significantly.

Future research should investigate further the dependence of uncertainty visualization design on ensemble data types and surrogate model capabilities. The trade-off in ensemble data size and surrogate model accuracy is a relevant consideration, as it will influence when each are utilized in a system. Finally, in this work we primarily focused on aleatory uncertainties, but including epistemic uncertainty is an additional complexity to consider for decision-making visualization systems.

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