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ANN-Based Inverse Goal-Oriented Design Method for Targeted Final Properties of Materials

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Abstract: Designing materials for targeted materials properties is the key to tackle the demands for personalized consumer products. The deficiency in the existing linear and nonlinear correlation methods attributed to simplifying assumptions and idealizations, nondeterministic simulations, and limited experimental data due to heavy computational time and cost, necessitates a design method that provides sufficient confidence to designers in decision making. To address this requirement, we propose, in this paper, an inverse goal-oriented materials design method supported by the design space exploration framework (DSEF). Keeping in view the accuracy and precision in the prediction confidence of machine learning-based methods, we developed an Artificial Neural Network based prediction model that supports DSEF. The proposed method for materials design can help designers to (1) explore PSPP spaces starting from end property requirements, (2) adjust the errors being propagated in the PSPP chain as well as in the predictions made by the model, and (3) timely adjust model parameters of the prediction model for accurate predictions. The efficacy of the method is illustrated for the hot stamping process to produce structural components from ultrahigh-strength steels (UHSS). The proposed method and prediction model are generic and applicable to any sequential manufacturing process to realize an end product.

Keywords: hot stamping; machine learning; integrated design; process–structure–property–performance; vertical and horizontal integration; decision-based materials design

1. Frame of Reference

Materials design is aimed at tailoring materials structure at various hierarchical levels (microstructural, atomic, etc.) in the chain of process–structure–property–performance (PSPP) to achieve desired properties and performance goals for a given application [1,2]. According to the definition of materials design “an activity that is top-driven, simulation supported, decision-based design of materials hierarchy to satisfy a ranged set of product-level performance requirements [2]”, to achieve the above-mentioned purpose requires systematic and adaptive designing of decision workflows in the chain of PSPP that are less sensitive to various types of variations and uncertainties involved [3]. Conceptually, the process involves the design of materials (process route, composition, etc.) to achieve trade-offs among conflicting criteria. To explore design set points that satisfy desired properties and performance goals, either experimental trial-and-error approaches or methods for model-based realization of engineered systems in simulation-based designs are employed to explore different phases/operations involved in a sequential manufacturing process. Experimental trial-and-error approaches are often very expensive in terms of both cost and time. The significant development of computational methods and tools based on first-principles and experimentations, and the enormous increase in the computing power of computers have enabled designers and engineers to simulate material properties and behavior in complex engineering applications with real-time conditions to avoid lengthy and expensive cycles of experimental trial-and-error methods. The deficiency in
the existing linear and nonlinear correlation methods attributed to simplifying assumptions and idealizations, nondeterministic simulations, and limited experimental data due to heavy computational time and cost, necessitates a design method that can give sufficient confidence to designers in decision making. This further necessitates extending designers’ abilities in the understanding and prediction of process behaviors in design by managing the uncertainties in decision workflows in the chain of PSPP [3].

Complex relationships exist between the processing inputs and the resulting microstructure, and between microstructural parameters and material properties. These relationships are difficult to manage by existing linear and nonlinear correlation methods attributed to simplifying assumptions and idealizations, non-deterministic simulations, and limited experimental data due to heavy computational time and cost. Because of these issues, uncertainty management is a significant challenge in the design of complex engineering systems with hierarchical, multiscale, and heterogeneous characteristics [4–7]. There have been many propositions from numerous researchers suggesting computational platforms from the perspective of decision-based design to support designers in design space exploration with an appreciative capture of uncertainty [8]. Choi et al. [9] categorized the uncertainties involved in the materials design process as Natural Uncertainty (NU), Model Parameter Uncertainty (MPU), Model Structure Uncertainty (MSU), and Propagated Uncertainty (PU). In response, several researchers put forward useful contributions addressing a single or combination of the uncertainties involved. For example, the Robust Concept Exploration Method (RCEM) [10] and its variances: RCEM with Design Capability Indices (RCEM–DCI) [11] and RCEM with Error Margin Indices (RCEM–EMI) [12], Inductive Design Space Exploration (IDEM) [9], and Concept Exploration Framework (CEF) [13,14], provide platforms to support design space exploration based on the compromise Design Support Problem (cDSP) construct. Some robust design methods and tools have also been developed to manage the uncertainties involved in the design process [15,16]. As mentioned above, all these platforms and contributions have employed the incomplete, incorrect, and infidel models that limit the confidence and freedom of designers in decision making. There is need for a robust, uniform model and method that can give sufficient confidence to designers to manage uncertainties involved in the chain of PSPP and make decisions with satisfying solutions. In this study, we identify, based on the discussion above, three aims that a materials design process should address: (1) guide designers from end property and performance goals to the processing parameters in an inverse, goal-oriented way, (2) provide sufficient freedom and space to designers to adjust errors at every decision node during the design process, i.e., manage propagated uncertainty, and (3) allow designers to timely adjust model parameters for accurate predictions, i.e., Manage Model Parameter Uncertainty (MPU) and Model Structure Uncertainty (MSU).

Keeping in mind the above challenges and targets, the following are the questions to be answered in order to achieve the desired outcome. Primary Research Question: How can the design spaces be explored and the mappings in the PSPP chain be coupled using machine learning?

- **Research Question 1**: How can the dataset of inputs and outputs for each mapping of the PSPP be obtained?
- **Research Question 2**: How can the small datasets to predict the outputs be accurately addressed?
- **Research Question 3**: Based on the phenomena, how can the flow of information (forward and backward) across the PSPP chain in the hot stamping process be established?
- **Research Question 4**: How can the uncertainty at each stage as well as the overall process be managed?

In this work we have attempted to address the three aims except MPU, which is the subject of our future work.

Due to the development of machine learning (ML) based methods, the complex, non-linear relationships can now be modeled efficiently and effectively [17]. ML-based methods
have the ability to capture functional relationships from data and knowledge without knowing the fundamental science-based mechanisms and relationships. Well-established ML-based models, in general, and ANN-based models, in particular, have been developed and employed for tailoring materials properties and design. Several examples can be found in the literature featuring success stories of the application of ML-based models and techniques in the materials design process in general [18–26] and particularly in the field of processing and manufacturing steel and other alloys [27–46].

Existing analytical and computational models and tools enable designers to efficiently solve standard forward problems, i.e., to predict properties and behaviors of particular materials under specific processing conditions. However, the methods to handle inverse problems are less well developed, i.e., to design or engineer new materials with desired properties and performance goals. Materials design problems using ML methods can be described by considering, given dataset (e.g., microstructure-property) obtained from physical experiments and/or computations based on first-principles [17,47,48], the best combinations of input parameters that possess the desirable output (e.g., microstructure or properties). Datasets can provide great opportunities for the application of ML-based methods or data-driven techniques to accelerate the tailoring of materials with desired properties.

This work focuses on seeking satisficing solutions that can perform well under uncertainty rather than optimal solutions, which perform poor when subjected to uncertainties. Optimal solutions perform well for a very narrow range, but when there is a shift in conditions, their performance suffers [13]. Therefore, designers are required to make decisions with satisficing solution set points that perform well enough under uncertainty. Through this work, a contribution is put forward to provide designers with an effective platform to make decisions in the “what if” scenarios to achieve satisficing solutions among the conflicting goals/requirements. To achieve this, an attempt is made to take advantage of the accuracy and precision in the prediction confidence of Artificial Neural Network (ANN) to address the issues discussed above. ANN-based models have the capability to learn any kind of functional relationship from experimental data within an arbitrary degree of accuracy, and this capability is not limited to a particular set or class of functional relationships. ANN-based models can steer engineering design decisions if it successfully and efficiently learns functional relationships during training and development using experimental data.

Keeping in view the requirements discussed above, the primary contribution of this work is an inverse, goal-oriented method supported by a Design Space Exploration Framework (DSEF). DSEF is further supported by the ANN-based prediction model, which is capable of capturing the complex, non-linear functional relationships in all spaces of the PSPP, i.e., process–structure (PS), structure–property (SP) and property–performance (PP). It starts directly from the end requirements and traces back the PSPP spaces in the inverse direction. The prediction model considers mechanical and thermal information successfully to predict phase distribution, microstructure, and end properties. For ANN-based prediction model development, due to the small number of data points in the datasets, a statistical technique (k−fold cross validation) has been utilized for optimal utilization of the data [49–55]. k−fold cross validation helped us develop a robust ANN model to avoid the issue of overfitting, and it also helped us to explore different network topologies for our prediction model. k−fold cross validation helped successfully encapsulate the localized variations in the prediction capability of the model in the experimental space and in PSPP spaces. It allowed us to generate customized bars for uncertainty in the predictions made by the model. After developing the prediction model, its capability to make accurate predictions was rigorously measured and analyzed by exposing the prediction model to completely new and independent data. The efficacy of the method is illustrated by exploring the design/solution of all the PSPP spaces of the hot stamping process. We illustrate in this work that ANN-based methods can provide a better platform for making decisions in the chain of PSPP and relieving the designers of the hectic efforts to integrate the incomplete, inaccurate, and infidel physical and empirical models that cause MPU, MSU, and PU in
decision workflows. The ML-based prediction model can help designers to timely address the variations at every decision node in the design process.

The outline of the paper is as follows. Section 2 presents a brief overview of the hot stamping process. Section 3 presents a description of the Design Space Exploration Framework (DSEF). Section 4 presents the ANN-based prediction model development and its validation. Section 5 presents an inverse goal-oriented design method for hot stamping. Section 6 presents the implementation of the proposed method and solution space exploration. Section 7 concludes our work with closing remarks.

2. The Hot Stamping Process

Hot stamping is a thermomechanical forming process with intended transformation both in microstructure and macrostructure. Figure 1 represents a basic hot stamping process. Hot stamping is a complex manufacturing process. The basic steps of hot stamping are as follows:

- Heating—Blank is heated up to the austenitization temperature. This temperature has significant influence on the blank properties, the processing time, and the cost-efficiency of hot stamping.
- Forming and Quenching
  - Forming—Provides pressing for macrostructure transformation and must be finished before the beginning of the martensite transformation.
  - Quenching—Immediately after finishing forming, the transformation from austenite into martensite occurs here. The morphologies of these microstructures (austenite and martensite) are very different and thus possess different mechanical properties.

In the automotive industry, the manufacturing of structural components from ultra-high-strength steels (UHSS) is rapidly increasing to enhance safety and reduce fuel consumption. Low form-ability and substantial spring-back put constraints on the formation of UHSS at room temperature. Therefore, hot stamping is the best alternative and has been widely used to date. The complexity of the hot stamping process originates from high working temperature and simultaneous quenching, and the need to control the processing parameters, during both phases, precisely to achieve desired phase fraction percentage and hence desired properties. Like other steels, Boron steel (22MnB5) in the austenite phase has low flow stress at elevated temperatures. This process has the capability to take advantage of this aspect of boron steel and produce parts with high tensile strength, minimum spring-back, and reduced sheet thickness.

Process designers must look for cost-effective solutions that help in decision making and improve the efficiency of the process. Hot stamping involves both materials design and structural design. Careful design of the hot stamping process can produce automotive structural parts with desired mechanical properties with acceptable quality, maximum output, and minimum cost subject to the limitations and constraints of the hot stamping mill. The challenges associated with the design of the hot stamping process are attributable
to the complex nature of the process, which involves a large number of processing parameters, complex relationships, constraints and bounds, and the hierarchical nature of PSPP relationships. In this work, we attempt to address some of these challenges by developing a design method supported by an ANN-based prediction model and design space exploration of the hot stamping process to realize an end product. The next section presents the Design Space Exploration Framework (DSEF).

3. Design Space Exploration Framework

We explain the DSEF proposed in this work. There are three stages in the DSEF to identify design alternatives/solutions and identify satisficing design solutions. Figure 2 presents the DSEF infrastructure. All three stages are explained below.

![Figure 2. Design Space Exploration Framework.](image)

A. **Goal Analysis**

The initial desired design space is defined in this stage. The design specifies the requirements for both control and noise factors for the end product, and their ranges are specified to achieve the requirements.

B. **Prediction Model Development and Model Evaluation**

Stage 2 consists of four steps:

**Step 1:** The designer identifies the parameters that influence the end product properties and performance. After parameter identification, an important step is to determine whether datasets are available. If already developed datasets are not available, physical simulations are needed to prepare a dataset with enough data points.

**Step 2:** Physical experiments are very expensive and time consuming to be carried out repeatedly. Therefore, some statistical techniques can be used if enough data points are collected as discussed in step 1. Statistical techniques will help in utilizing limited data optimally for learning functional relationships.

**Step 3:** Once the influential parameters are identified and the datasets are prepared, a machine learning-based model is developed to capture the functional relationships between input and output parameters using the information in the dataset. Prediction model development has been explained in detail in Section 5.

**Step 4:** After developing the model, it is analyzed and validated for its performance to check its generalization capability and robustness. After finishing stage 4 and training the model using the dataset, the next step is to explore the design space.
C. Solution Space Exploration

Once the ranges for the end properties are identified by the designer and the ANN model is executed for both datasets, i.e., input and test datasets, the solution space is explored and compared with the requirements. Solutions are accepted if requirements are satisfied. If not, a designer can recommend changes in either the influential parameters or the overall end goal requirements.

In the next section, we describe the base algorithm for our work, the ANN, with its applications in the fields of material processing and manufacturing.

4. ANN-Based Prediction Model Development and Validation

4.1. Prediction Model Development

The most critical part of the prediction model is the availability or development of the dataset. If physical experiments are carefully carried out and the generated dataset contains a variety of data that cover almost all the scenarios and are not biased to any specific situation, the prediction model can capture functional relationships efficiently. Some machine learning algorithms are better suited for a particular type of dataset, and some are useful for other types of datasets. Therefore, to achieve higher accuracy, it is important to choose the right machine learning algorithm. If properly modeled, machine-learning-based models have better accuracy than physical or empirical models. In this work, we applied an ANN as the base algorithm for the prediction model proposed.

An ANN is a mathematical model that can generalize previous experiences/observations to new ones in a similar fashion as to how human brains work. In this work, we propose a multilayered, feed-forward ANN with a back-propagation ANN model [56]. For our prediction model, an ANN topology was selected that consists of one input layer, one output layer, and two hidden layers along with a sigmoid activation function. Such a model can learn any complex, nonlinear multivariate functional relationship [56–58].

\[
f(x) = \frac{1}{1 + e^{-x}}
\]  

(1)

In the PSPP spaces of hot stamping, there are respective numbers of nodes in the input and output layers for each space. The values of input and output parameters for each space of the hot stamping process are shown in Table 1. In this work, our target is to demonstrate our proposed method for process–structure and structure–property spaces of hot stamping. Property–performance space is the subject of our future work. In this work, the classic back-propagation algorithm was used for training and developing our model [56].

4.1.1. Weights and Weight Initialization

In an ANN, a set of weights is attached to the neurons in the hidden layer(s) and output layer. Initial weights are initialized randomly, and these initial values determine the starting point where the ANN starts the search to find the error minima during its training, where different random initializations mean different starting points. Due to different random initializations, the ANN model follows a different path each time during its training to arrive at different error minima, even though they are trained using the same data and have the same ANN topology. Therefore, to incorporate the effect of the random initialization, we applied the five different random weight initialization techniques given in Table 2. When the model is run, the generated output is used to calculate the difference between predicted values and actual values. The weights are then updated iteratively to minimize the error. The iterations continue until the error is minimized. This is what is called the learning process during ANN-based modeling.
Table 1. Parameters involved in the PSPP chain of the Hot Stamping Process.

| PSPP                  | Input Parameters                                                                 | Output Parameters                                      |
|----------------------|----------------------------------------------------------------------------------|--------------------------------------------------------|
| **Heating**          | a. Initial Microstructure                                                       | a. Austenite phase fraction values (%)                  |
|                      | b. Heating Rate                                                                 | b. Ferrite phase fraction values (%)                    |
|                      | c. Soaking Temperature                                                           | c. Pearlite phase fraction values (%)                   |
|                      | d. Soaking Time                                                                  |                                                        |
| **Process–Structure**|                                                                                  |                                                        |
|                      | a. Austenite Phase Fraction Value (%)                                            | a. Martensite phase fraction values (%)                 |
|                      | b. Various temperature ranges to which the blank is heated                       | b. Bainite phase fraction values (%),                   |
|                      | c. Various starting temperatures for deformation                                 | and                                                   |
|                      | d. Cooling Rate                                                                  | c. Ferrite phase fraction values (%)                    |
|                      | e. Various deformation amounts (%)                                               |                                                        |
| **Forming and Quenching** |                                                                                  |                                                        |
|                      | a. Martensite phase fraction values (%)                                          | a. Hardness                                            |
|                      | b. Bainite phase fraction values (%)                                             | b. Tensile Strength                                    |
|                      | c. Ferrite phase fraction values (%)                                             |                                                        |
| **Structure–Property** |                                                                                  |                                                        |
|                      |                                                                                  |                                                        |

Table 2. Random Initialization Methods.

| Initialization Methods                                      | Description                                               |
|------------------------------------------------------------|------------------------------------------------------------|
| (1) Conventional Random Initialization                      | \( W^l = \text{np.random.randn}(l - 1, l) \)               |
| (2) He Random Initialization [59]                           | \( W^l = \text{np.random.randn}(l - 1, l) * \text{np.sqrt}(2/l - 1) \) |
| (3) A variance of the Random Initialization Proposed by He et al. [59] | \( W^l = \text{np.random.randn}(l - 1, l) * \text{np.sqrt}(2/(l - 1 + 1)) \) |
| (4) Xavier Random Initialization [60]                       | \( W^l = \text{np.random.randn}(l - 1, l) * \text{np.sqrt}(1/l - 1) \) |
| (5) Normal (Gaussian) Distribution                          | \( W^l = \text{np.random.normal}(\text{mean}, \text{sigma}, (l - 1, l)) \) |

4.1.2. Division of the Datasets

As the number of data points in the datasets for each space of the hot stamping was small, we divided the datasets into an input dataset and test dataset. Initially, 80% of the data points in the overall dataset were allocated to the input dataset for training the model, while 20% were allocated to the test dataset. We exploited statistical techniques to optimally utilize limited data. We utilized the k-fold cross-validation (k-fold CV) technique, which has proven to be very useful for small datasets [56]. k-fold CV provides the opportunity for each data point in the input dataset to be used for cross-validation at least one time and for training \( k \) one time [56], as shown in Figure 3.

In this work, the input dataset consisted of 40 data points, while the test dataset contained 10 data points. Fourfold cross-validation was employed on the input dataset to generate distinct combinations of the training and CV datasets. This helps to prevent overfitting and ensure optimal utilization of the input data. The input dataset contained 30 points for training and 10 data points for cross-validation.
In this work, the input dataset consisted of \( k \times w \), which was different because each step has a different number of input and output parameters. To incorporate the effect of both network topology and random initialization, we employed the rule of thumb method, which says “the number of neurons in hidden layers should be between the size of the input layer and the size of output layer” [57].

### 4.1.3. Number of Neurons in Hidden Layer

The number of neurons in hidden layers is a key aspect in deciding ANN topology because of its significant influence on the final output. Hidden layers with a small number of neurons result in underfitting because they cannot adequately detect the functional relationships in a complex dataset. An ANN model with too many neurons in hidden layers can simulate any complex functional relationships but at the expense of high computational cost. However, excessive neurons in hidden layers can result in overfitting. A higher number of neurons in hidden layers results in a higher number of weights attached, which increases the dimensions of the hypothesis space in which the model looks for minimum error. Additionally, higher dimensions of the hypothesis space complicate the error surface with many suboptimal local minima, which makes it difficult to find optimal error minima during the training. Furthermore, due to random initialization of the ANN model, it is very difficult to find the optimal number of neurons in hidden layers. In this work, we employed the rule of thumb method, which says “the number of neurons in hidden layers should be between the size of the input layer and the size of output layer” [57].

### 4.1.4. Final ANN Model

Network topology and random initialization both significantly influence the performance of the ANN. To incorporate the effect of both network topology and random weights in our model, the number of neurons in hidden layers was made to keep swapping among different numbers \( (1, 2, 3, \ldots, n) \). Hence, for two hidden layers, swapping the number of neurons among \( n \) numbers gave rise to a total of \( c = n \times n \) combinations, as shown in Table 3. All these \( c \) combinations of network topologies were trained on \( k \) sets of training and CV datasets generated through \( k \)-fold CV, resulting in \( c \times k \) ANN models. Each of these models was initialized with different random weight initialization methods \( (1, 2, 3, \ldots, w) \). The random initialization methods used are shown in Table 2. Finally, we have \( N = c \times k \times w \) models that were trained on the input dataset. The number of iterations was different because each step has a different number of input and output parameters, and for each step, a specific number of iterations was determined when the CV error was at a minimum to avoid overfitting of the model. A generalized schematic of the ANN has been given as Figure 4.

The default learning rate in the ANN was chosen during the gradient descent in the back-propagation algorithm because the stopping criteria were the number of iterations and, as established separately for each step, how many iterations were sufficient for minimum CV error. Table 4 shows parameters of the proposed ANN model.
Table 3. Summary of the Models Generated.

| PSSP                           | Dataset | Input Dataset | Test Dataset | K-Fold CV | Number of Nodes in Hidden Layers | Random Initialization Methods | Total Models N |
|-------------------------------|---------|---------------|--------------|-----------|----------------------------------|-----------------------------|----------------|
| Process–Structure             |         |               |              |           |                                  |                             |                |
| Heating                       | 60      | 48            | 12           | 4         | 2, 3, 4 = 3 No’s                 |                             | 180            |
| Forming and Quenching         | 50      | 40            | 10           | 4         | 3, 4, 5 = 3 No’s                 |                             | 180            |
| Structure–Property            | 50      | 40            | 10           | 4         | 2, 3, 4 = 3 No’s                 |                             | 180            |

The default learning rate in the ANN was chosen during the gradient descent in the backpropagation algorithm because the stopping criteria were the number of iterations and, as established separately for each step, how many iterations were sufficient for minimum CV error.

Table 4. Parameters of the ANN model for all PSPP spaces.

| Parameters                        | Step 2                      | Step 3.1                     | Step 3.2                     |
|-----------------------------------|-----------------------------|------------------------------|------------------------------|
| Number of Layers                  | Input Layer: 1,             | Input Layer: 1,             | Input Layer: 1,             |
|                                   | Output Layer: 1,            | Output Layer: 1,            | Output Layer: 1,            |
|                                   | Hidden Layers: 2            | Hidden Layers: 2            | Hidden Layers: 2            |
| Number of Neurons in each Layer   | Input layer: 2,             | Input layer: 3,             | Input layer: 1,             |
|                                   | Output Layer: 3,            | Output Layer: 5,            | Output Layer: 3,            |
|                                   | Hidden Layer: 2,3,4         | Hidden Layer: 3,4,5         | Hidden Layer: 2,3,4         |
| Weight Initializations            | 5                           | 5                            | 5                            |
| Learning Rate                     | Default                     | Default                      | Default                      |
| Activation Function               | Sigmoid                     | Sigmoid                      | Sigmoid                      |
| Number of Iteration               | 10,000                      | 12,000                       | 10,000                       |
4.1.5. Uncertainty in Predictions

$N$ number of results are generated corresponding to $N$ models when all the models are trained using the input dataset. The final result is the mean of all these $N$ results.

$$\text{Final output} = \frac{\sum \text{(Predictions made by all models in } N)}{\text{Number of models in } N} = \frac{1}{N} \sum_{i=1}^{N} \text{output}_i \quad (2)$$

Each of the $N$ models makes predictions that are moderately different from the predictions made by other models because each model results in different error minima, even though all the $N$ models are being trained to capture the same functional relationship from the information in the input dataset. This variation in results can be represented by a standard deviation $\sigma$ in the predictions. Uncertainty bars are incorporated to show the uncertainty/variations in predictions made by the $N$ models. Standard deviation $\sigma$ in the predicted values by $N$ models was determined, and bars for the uncertainty were drawn using the following formula:

$$\text{Uncertainty Bar} = \pm 2 \times \sigma \quad (3)$$

Because 95% of the observations/predictions fall within two standard deviations from the mean value, the factor of two was selected. Each of the predictions made by $N$ models take the following form:

$$\text{Mean Value of each Prediction} \pm 2 \times \sigma \quad (4)$$

This statistical approach helped us to identify localized variations in our model predictions. Uncertainty bars are shown by the blue line on each predicted value in Figures 6–11. The blue lines show the deviations in the predicted values.

4.2. Prediction Model Validation

The most important value of an ANN model is its generalization capability—the ability to forecast the unknown test data. Once the model is developed, it is mandatory to analyze and validate its performance rigorously by exposing it to the data present both in the input and test datasets. Model validation judges the generalization capability of the model for completely new data. In this work, model performance was validated by calculating the loss function. Predicted values ($\hat{Y}_i$) and actual output values ($Y_i$) in the input and test datasets are compared to calculate the loss function. The minimum loss function is the maximum robustness and reliability of the model. The Root Mean Square Error (RMSE) has been used as the loss function.

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (Y_i - \hat{Y}_i)} \quad (5)$$

5. Designing Hot Stamping Process—An Inverse Goal-Oriented Design Method

As mentioned earlier, the aim of this work is to develop an inverse goal-oriented method that is independent of the forward flow. The method implemented in this work does not need to establish a forward flow of information in the PSPP chain. It can lead the designer directly from the requirements to the identification of the process parameters in an inverse direction. The information flow for this goal-oriented method will be elaborated on, as depicted in Figure 5. The flow of information starts with end product goals desired for the product and process. The preceding stages are explored to identify solution set points that satisfy the end goals. All steps for the method are explained below.
Step 1 Performance–Property Space: Step 1 involves identification of the end product performance goals (stiffness, reliability, and minimum mass). Performance parameters are dependent upon the material properties. Upon exercising the ANN model in step 1 and exploring the solution space (using stage C of DSEF), the ranges for hardness, tensile strength, and density are identified that satisfy the performance goals. These ranges are communicated to step 2 as design information.

Step 2 Property–Microstructure Space: Step 2 has the target goals for material properties (hardness, tensile strength, and density) received from step 1. By exercising the ANN model in step 2 and exploring the solution space (using stage C of DSEF), the combinations for martensite, bainite, and ferrite phase fraction values are identified that satisfy the requirements for the material properties. These combinations are communicated to step 3.1 as design information.

Step 3.1 Microstructure–Process Space: Step 3.1 receives target goals for martensite, bainite and ferrite phase fraction values from step 2. Following a similar procedure, the combinations of the austenite phase fraction values, soaking temperature, deformation amount, cooling rate, and deformation temperature are identified that satisfy the target goals of the microstructure. Among the design information generated in step 3.1, only target goals for austenite are communicated to step 3.2.

Step 3.2 Microstructure–Process Space: Following the same process and after exploring the solution space of heating phase parameters, the combinations of heating rate, soaking temperature, and soaking time are identified that satisfy the target goals of austenite phase fraction values.

The inverse, goal-oriented design method described above is generic for any manufacturing process that involves multiple processes in sequence. In the current work, we skipped step 1 because of the unavailability of the dataset to learn the functional relationship between performance goals and material property. We demonstrated the efficacy of the design method for steps 2, 3.1 and 3.2. In the next section, we provide in detail the implementation of our proposed method.

6. Implementation of the Proposed Method and Solution Space Exploration

In this section, we detail the implementation of our proposed model and method. This work does not cover step 1 (performance–property), and we started with step 2, as shown in Figure 6. After running our model for each space, the solution space was explored to identify the solution set points that satisfy the requirements for each module. For solution space exploration, the parameters involved in each module were normalized between 0 and 1. The 0 value corresponds to the minimum value of a parameter, while the 1 value...
corresponds to the maximum value. Each parameter value was normalized using the maximum value of that parameter in the output results using the following expression.

\[ r_{ij} = \frac{p_{ij}}{\max_j p_{ij}} \]  

(6)

where \( r \) has values in the range of 0–1. \( p_{ij} \) the value of parameter \( i \) in the \( j \)-th row, and \( \max_j p_{ij} \) shows the maximum value of the parameter \( i \) in the \( j \)-th row.

**Figure 6. Inverse Flow of Information in Hot Stamping (step 1 skipped).**

**Step 2 Property–Microstructure Space:** Step 2 of the information flow involves identification of the target goals for material properties, hardness, and tensile strength. Density was not included because no material removal or addition was involved; therefore, only two material properties were considered. The dataset for property–microstructure space was not available, so we took advantage of the fact that each individual phase fraction has its own hardness value. For each microstructure combination in the dataset obtained from [48], we obtained values for hardness and tensile strength using established empirical formulae [50]. For each individual phase fraction, we multiplied its hardness by its percentage, and then the mean was calculated for the summation of all the phase fractions, as shown in Table 5.

**Table 5. Illustration of the Method followed with the Generate Dataset for Step 2.**

| Phase Fraction % | Unit Hardness HV | Overall Hardness |
|------------------|------------------|------------------|
| Martensite %     | 24               | 435              |
|                  | (10,440 + 6600 + 10,800)/100 = 278.40 HV |
| Bainite %        | 22               | 300              |
|                  | 278.40 * 3.45 = 980 MPa |
| Ferrite %        | 54               | 200              |
|                  | 6600             |
| Mean Hardness    | 24               | 10,440           |
|                  | 6600             |
| Tensile Strength | 278.40           | 980              |

For a microstructure combination of 24% martensite, 22% bainite, and 54% ferrite, the corresponding values of hardness and tensile strength are 278.4 HV and 980 MPa, respectively. We generated 50 data points using the data from the dataset of [48]. The
dataset for step 2 contains hardness and tensile strength as input parameters and phase fractions of martensite, bainite, and ferrite as output parameters. The ANN parameters for step 2 are shown in Table 4. After running the model for the dataset, the results were plotted to visualize the predicted output by our model and the actual output in the dataset, as shown in Figures 7 and 8 for the input dataset and test dataset, respectively. Additionally, loss functions were calculated to demonstrate the agreement of closeness between predicted output and actual output for both the input dataset and test dataset. Values of the loss function calculated for step 2 are shown in Table 6.

Table 6. Loss Functions for Step 2 (RMSE).

| Data Type   | Input Dataset | Test Dataset |
|-------------|---------------|--------------|
| Martensite  | 5.58          | 6.31         |
| Bainite     | 4.17          | 1.73         |
| Ferrite     | 4.90          | 5.42         |

For solution space exploration, the requirements for mechanical properties were specified as shown in Table 7. The requirements are provided in the form of ranges that satisfy a given engineering design problem. Upon mapping these requirements with the results for the ANN model, a feasible region was identified as shown by the shaded area in Figure 9. The x-axis of Figure 9 represents the number of data points in the output results. The y-axis represents the combinations of the microstructure at each data point. The red line represents the corresponding tensile strength of each microstructure combination. All microstructure combinations were plotted against the ascending order of the tensile strength so that the feasible region (green rectangular) could be identified. The ascending order allowed us to easily identify the lower and upper limits of the tensile strength requirements. The data points in this feasible region were the microstructure combinations that satisfied the tensile strength requirements. Tensile strength was selected because the target for the hot stamping process is to obtain the best tensile strength.

Table 7. Requirements on Mechanical Properties (Step 2).

| Limits     | Final Requirements |
|------------|--------------------|
| Hardness (HV) | Tensile Strength (MPa) |
| Lower Limit | 350                |
| Upper Limit | 430                |
| Lower Limit | 1250               |
| Upper Limit | 1500               |

Figure 7. Predicted Output and Actual Output Comparison for Step 2 (For Input Dataset).

Figure 8. Predicted Output and Actual Output Comparison for Step 2 (For Test Dataset).
Table 6. Loss Functions for Step 2 (RMSE).

| Error/Data Type | Input Dataset | Test Dataset |
|-----------------|---------------|--------------|
| Root Mean Squared Error % (RMSE) | Martensite % | 5.58 | 6.31 |
|                 | Bainite %     | 4.17 | 1.73 |
|                 | Ferrite %     | 4.90 | 5.42 |

For solution space exploration, the requirements for mechanical properties were specified as shown in Table 7. The requirements are provided in the form of ranges that satisfy a given engineering design problem. Upon mapping these requirements with the results for the ANN model, a feasible region was identified as shown by the shaded area in Figure 9. The x-axis of Figure 9 represents the number of data points in the output results. The y-axis represents the combinations of the microstructure at each data point. The red line represents the corresponding tensile strength of each microstructure combination. All microstructure combinations were plotted against the ascending order of the tensile strength so that the feasible region (green rectangular) could be identified. The ascending order allowed us to easily identify the lower and upper limits of the tensile strength requirements. The data points in this feasible region were the microstructure combinations that satisfied the tensile strength requirements. Tensile strength was selected because the target for the hot stamping process is to obtain the best tensile strength.

Table 7. Requirements on Mechanical Properties (Step 2).

| Limits       | Final Requirements |
|--------------|---------------------|
|              | Hardness (HV) | Tensile Strength (Mpa) |
| Lower Limit  | 350 | 1250 |
| Upper Limit  | 430 | 1500 |

Figure 9. Feasible Region for Microstructure Parameters.
The set of feasible phase fraction values of martensite, bainite, and ferrite were identified as shown in Table 8. The loss function for step 3.1 was calculated as shown in Table 9. The Table 8 shows that the minimum phase fraction of martensite is 55.99%, while the maximum is 89.99%. Similarly, for bainite and ferrite, the minimum phase fractions are 9.99% and 4.3%, while the maximum phase fractions % are 16.55% and 23.55%, respectively. These identified phase fraction combinations satisfy the requirements specified by the designer. These combinations are converted to ranges as shown in Table 10. The design information, these phase fraction combinations in the form of ranges, and is communicated to step 3.1 as requirements or targets.

**Table 8. Phase Fraction Combinations Satisfying the Requirements on Mechanical Properties.**

| Microstructure Combinations Identified after Solution Space Exploration |
|---------------------------------------------------------------|
| Martensite | Bainite | Ferrite |
|------------|---------|---------|
| 55.99 | 16.55 | 23.50 |
| 67.50 | 14.74 | 8.02 |
| 75.82 | 14.67 | 7.80 |
| 78.99 | 15.71 | 4.99 |
| 80.02 | 12.05 | 4.30 |
| 80.99 | 13.62 | 4.99 |
| 83.55 | 12.90 | 5.55 |
| 86.52 | 11.02 | 6.77 |
| 89.70 | 11.40 | 6.27 |
| 87.69 | 9.99 | 5.99 |
| 89.99 | 10.98 | 6.03 |
| 88.99 | 10.74 | 5.33 |

**Table 9. Loss Functions for Step 3.1.**

| Error | Data Type         | Training Data | Test Data |
|-------|-------------------|---------------|-----------|
| RMSE  | Austenite %       | 1.97          | 2.58      |
|       | Temperature at t = 0 | 5.54          | 9.19      |
|       | Cooling Rate CR   | 4.74          | 5.48      |
|       | Deformation Amount | 2.03          | 1.79      |
|       | Deformation Time  | 6.93          | 7.03      |

**Table 10. Requirements on Microstructure Combinations.**

| Limits | Requirements for Step 3.1 |
|--------|---------------------------|
|        | Martensite % | Bainite % | Ferrite % |
| Lower  | 60           | 10        | 4         |
| Upper  | 90           | 17        | 24        |

**Step 3.1 Microstructure–Process Space (Forming and Quenching Phase):** The thermal and mechanical processing conditions during forming and quenching define the complex microstructure mixture of martensite, bainite, and ferrite [61–66]. The dataset for this step was obtained from [48], which involve phase fraction combinations of martensite, bainite, and ferrite as input parameters, and the output parameters are temperature at t = 0, austenite %, cooling rate CR, deformation amount and deformation temperature. The same process was
followed as in step 2 with ANN parameters given in Table 4 for step 3.1. Figures 10 and 11 present visualizations of the predicted output and actual output for both the input dataset and test dataset, respectively.

Figure 10. Predicted Output and Actual Output Comparison for Step 3.1 (for Input Dataset).

The requirements on the microstructure combinations were received from step 2 as shown in Table 10. The microstructure requirements are provided in the ranges that satisfy mechanical property requirements. Upon mapping these requirements with the results for the ANN model, a feasible region was identified as shown by the green rectangular area in Figure 12. The same procedure was followed to draw Figure 12. The red line represents the martensite phase fractions for each processing parameter combination. The martensite phase fraction was selected because the target for the forming and quenching phase is always to achieve as much martensite as possible. From the feasible region, a set of feasible values of austenite %, temperature at $t = 0$, cooling rate CR, deformation amount, and deformation temperature were identified as shown in Table 11. These identified combinations of the processing parameters for forming and quenching satisfy the microstructure requirements received from the previous step. After identifying the combinations of the processing parameters for the forming and quenching phase, i.e., austenite %, temperature at $t = 0$, cooling rate CR, deformation amount, and deformation temperature, the design information on austenite % is communicated to step 3.2. The austenite % phase fraction is the target for step 3.2.
Figure 11. Predicted Output and Actual Output Comparison for Step 3.1 (for Test Dataset).

Table 11. Processing Parameter Combinations Satisfying Microstructure Requirements.

| Temperature at \(t = 0\) | Austenite % | Cooling Rate | Deformation Amount | Deformation Temperature |
|--------------------------|-------------|--------------|--------------------|------------------------|
| 1123.87                  | 94.99       | 57.93        | 13.80              | 1064.08                |
| 1121.85                  | 96.02       | 62.67        | 12.84              | 1067.72                |
| 1118.08                  | 95.01       | 58.26        | 11.55              | 1065.76                |
| 1122.25                  | 96.49       | 57.93        | 17.28              | 1063.07                |
| 1121.29                  | 95.51       | 52.32        | 18.73              | 1063.04                |
| 1117.11                  | 97.44       | 71.48        | 11.28              | 1050.18                |

Step 3.2 Microstructure–Process Space (Heating Phase): The phase fraction % of martensite after forming and quenching is greatly affected by the phase fraction % of austenite. The formation of austenite during the heating phase is very influential upon the final properties of the product produced by hot stamping. The dataset for this step was obtained from [47], which involves the austenite phase fraction % as an input parameter, while the output parameters are heating rate \(HR\), soaking temperature, and soaking time. The same process was followed as for previous steps with ANN parameters given in Table 4 for step 3.2. Figures 13 and 14 present plots of the predicted output and actual output for both
the input dataset and test dataset, respectively. The loss function for step 3.2 was calculated as shown in Table 12.

![Feasible Solution Region for Step 3.1](image)

**Figure 12.** Feasible Region of the Processing Parameters (Forming and Quenching).

![Predicted Output and Actual Output Comparison for Step 3.2 (for Input Dataset)](image)

**Figure 13.** Predicted Output and Actual Output Comparison for Step 3.2 (for Input Dataset).
For solution space exploration, the requirements on the austenite phase fraction % are received from step 3.1 as shown in Table 13. The austenite phase fraction requirements are provided in the ranges. Upon mapping these requirements with the results for the ANN model, a feasible region is identified as shown by the green rectangular area in Figure 15. Following the same procedure as in the last step, a plot was drawn. The redline in Figure 15 represents the austenite phase fraction values for each processing combination of the heating phase. Austenite was selected because the target for the heating phase is always to achieve as much austenite as possible. From the feasible region, a set of feasible values of heating rate $HR$, soaking temperature, and soaking time were identified as shown in Table 14. These identified combinations of the processing parameters for the heating phase satisfy the austenite phase fraction requirements received from step 3.1.

Table 13. Austenite Phase Fraction Requirements.

| Limits     | Requirements from Step 3.1 | Austenite Phase Fraction % |
|------------|----------------------------|----------------------------|
| Lower      | 95                         | 95                         |
| Upper      | 98                         | 98                         |

After execution of our model for steps 2, 3.1 and 3.2 and exploring the solution space, the design set points for each space were identified that satisfy the requirements for each space. The method proposed and demonstrated for the hot stamping process can help designers with respect to (1) guidance from end goals to the processing goals, (2) adjustment of the variations and error being propagated, and modifications in model parameters, to...
explore the possibilities in achieving any desired set of properties for a product that are less sensitive to variations and satisfy the design performance/requirements. The method is robust in the sense that requirements are specified in ranges, and the corresponding processing or microstructure parameters identified are also in ranges. Hence, the designer has the freedom to adjust the ranges to minimize the effects of uncertainty, according to the available manufacturing facility available.

Figure 15. Feasible Region for Processing Parameters (Heating Phase).

Table 14. Processing Parameters (Heating) Combinations Identified After Solution Space Exploration.

| Combinations of the Processing Parameters (Heating Phase) Identified after Solution Space Exploration |
|---------------------------------|----------------|----------------|
| Heating Rate | Soaking Temperature | Soaking Time |
|----------------|----------------|----------------|
| 2.83            | 1104.89          | 11.19          |
| 9.35            | 1105.03          | 11.41          |
| 19.83           | 1104.89          | 11.19          |
| 24.99           | 1104.89          | 11.19          |
| 12.98           | 1106.80          | 11.50          |
| 9.89            | 116.80           | 11.50          |

A comparison of the predicted output with the actual values present in the dataset shows that our proposed ANN model has acceptable generalization capability. The predicted values could be added to the actual dataset, once validated experimentally, for deeper and further research. Another important observation is the simplicity and straightforwardness of the proposed Design Space Exploration Framework (DSEF). The DSEF can help the designer to start straightway from the end properties and trace back the PSPP spaces to realize the end product in a systematic manner in less time and in an efficient way.

In our current work, standard deviation was employed for uncertainty in prediction. To incorporate more accuracy and precision, acceptable margins of error can be employed.
as a stopping criterion for iteration. Model Parameter Uncertainty (MPU), not considered in our current work, is one of the potential areas for research and could enhance targeted material properties if properly managed. This is the subject of our future work.

7. Closing Remarks

This work follows two aims: first, to develop an inverse, goal-oriented design method for materials design supported by a solution exploration framework; and second, to develop an ANN-based prediction model that can predict output parameters in each space of the PSPP chain using limited or small datasets with better accuracy. The inverse design method is supported by the Design Solution Exploration Framework (DSEF). Apart from solution exploration, the DSEF helps designers to analyze solutions at each step rather than at the end of the whole process, thus allowing designers to make timely modifications in the end goals and requirements and thereby saving enough time during the computation and design process. The proposed method helps designers start directly from the specification of the end goals and by mapping these goals inversely with the microstructure and then against the processing parameters to explore solution space and identify solution ranges that satisfy the end goals.

A prediction model has been developed using a feed-forward Artificial Neural Network with a back-propagation algorithm. The model has better performance over all the spaces of the PSPP and is able to encapsulate complex functional relationships effectively, resulting in a close and accurate agreement between the actual output values in the dataset and the predicted output values. Performance of the prediction model suggests that ML-based methods (e.g., ANN-based models) could provide better platform for making decisions in the chain of PSPP. The efficacy of the method has been demonstrated by an integrated exploration of the solution set points needed to design the hot stamping process. The proposed method is generic and can be effectively applied to any manufacturing process involving a series of processes in sequence. We plan to incorporate other optimization techniques and machine learning models along with ANN to make our model more robust in the future.

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