

AI-Driven Autonomous Artifacts Inverse Design of Personalized Drug Delivery Artifacts for Healthcare Support in Special Education Populations

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ABSTRACT:

The growing need for personalized healthcare solutions for individuals with specific educational needs has inspired researchers to develop innovative drug delivery solutions for these populations. An autonomous design framework utilizing generative intelligence, inverse design, and interpretable machine learning can be used to develop personalized drug delivery artifacts. This framework considers the relationship between the characteristics of the patient, the drug delivery artifact components, and the desired therapeutic objectives to produce customized drug delivery systems. Generative AI can be used to create different drug delivery systems, and surrogate models can evaluate the performance of these systems. Inverse design techniques can be used to generate these artifacts to meet the objectives of the patient and the drug delivery system. Kolmogorov-Arnold Networks (KANs) can be used to create surrogate models to assess the performance of these drug delivery systems. These models can consider multiple objectives for the customized drug delivery systems, such as efficacy, accessibility, manufacturability, robustness, and cost-effectiveness. The results of these models can help develop novel healthcare solutions that can be applied to populations with special

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educational needs. The information obtained from these personalized drug delivery systems can help researchers and developers better understand the potential use of generative intelligence, inverse design, and explainable AI in the development of drug delivery systems that can cater to specific groups of patients with special needs in order to better provide healthcare to these populations.

Keywords: AI, Healthcare Support, Special Education.

1. Introduction

Artificial intelligence (AI) is rapidly transforming the various aspects of human creativity. Within the field of artifact creation, ai autonomous systems are beginning to propose and create artifacts that have the same intention and capability as their human creators. Currently, most artifacts are crafted by their artisans in accordance with certain goals and objectives of those artisans. The artisan can propose the artifacts that are to be created, the components of those artifacts, and the performance that the artifacts are to exhibit. While this process is effective in creating artifacts with the desired performances, the artisans are often limited in both the number of artifacts that they can propose, and in the optimality of those performances of the artifacts that they create.

Generative design is one concept that has significantly contributed to the abilities of autonomous systems to create artifacts with diverse performance criteria. Generative aesthetics is one method by which autonomous systems can propose artifacts with diverse designs for their components and functions. However, most generative methods do not include any step for evaluating the proposed artifacts for their potential performance, limiting their ability to effectively create artifacts relative to artisans.

Inverse design is another method by which autonomous systems can propose the performance that they desire from the artifacts that are created, and enable the system to determine the artifacts and their components that will achieve those performances. Inverse design methods are already implemented in various engineering fields. However, these methods are limited to the search

spaces for artifacts that are pre-defined within those engineering fields, preventing them from utilizing the diverse artifacts that can be created with generative models.

The integration of the concepts of generative aesthetics and inverse design represents a significant change in the creation of autonomous systems for the proposing of artifacts and their performances. While generative models have heretofore been utilized to propose artifacts and their components, inverse optimization methods can evaluate those proposed artifacts and adjusting their components to optimally achieve the performances of those artifacts. Thus, integrating these concepts allows for the shift from creating artifacts to creating autonomous systems that are able to create those artifacts.

AI models, such as Kolmogorov-Arnold Networks (KANs) have the ability to learn the complex nonlinear relationships between variables, which can be beneficial to the evaluation of artifacts. Furthermore, KANs are different from conventional black-box neural networks, and their benefits are applicable to the evaluation of artifacts created by autonomous systems. Additionally, the use of multi-objective models to evaluate artifacts for their efficiency, robustness, and aesthetic criteria enables the evaluation of artifacts in accordance with the goals that the artisans have for those artifacts.

Through developing an ai-driven computational framework that incorporates the elements of generative aesthetics and inverse design, autonomous systems will be able to propose artifacts that contain diversity in their components, designs, and performances, as well as ensure that

each artifact optimally performs according to the goals that are established for each individual artifact.

Literature Survey

The concept of computational design has its roots in the classical approaches to optimization techniques for structural design. For instance, Sigmund [1] described methods for topology optimization. These types of methods have been applied to new areas of research, such as the use of inverse design techniques for photonics, which were described by Molesky et al. [2]. Furthermore, Jensen and Sigmund [3] applied topology optimization methods to nanophotonic systems and demonstrated the effectiveness of these approaches for electromagnetic design.

The integration of machine learning techniques into the process of inverse design has led to developments in the area of nanophotonic inverse design, such as those proposed by Peurifoy et al. [4]. Additionally, others have explored the use of machine learning techniques for the discovery of new materials, as described by Liu et al. [5].

Various efforts have been made to employ surrogate modeling methods for the evaluation of designs that have been found through the application of inverse design. For instance, Rasmussen and Williams [6] described the use of Gaussian Processes for surrogate modeling. Additionally, other methods for surrogate modeling have been published, such as polynomial chaos methods by Xiu and Karniadakis [7]. Furthermore, the use of neural networks has also been published for surrogate modeling efforts due to the universal approximation property of neural networks [8]. For instance, Raissi et al. [9] published on the development of physics-informed neural networks, as well as others that have published on the use of deep learning surrogate models for nanophotonic systems [10].

Various efforts have been made for the modeling of multi-objective optimization problems. For instance, Deb et al. [11] published on the NSGA-II algorithm, which has been well-known in the field of optimization. Coello [12] reviewed the history of the development of multi-objective optimization

algorithms. Additionally, Marler and Arora [13] reviewed the methods for solving multi-objective optimization problems that arise within engineering. Furthermore, approaches to generative modeling for inverse design have been published by Sanchez-Lengeling and Aspuru-Guzik [14], for instance in the context of employing machine learning techniques to discover new molecular compounds.

Various approaches to autonomous design systems have been made. For instance, Nikolaev et al. [15] published on autonomous materials research. Deep learning, one of the main areas of development for AI, has been developed by individuals such as LeCun et al. [16] and Schmidhuber [17]. Deep learning models have been applied to the modeling of digital twins of manufacturing systems by authors such as DebRoy et al. [18].

Classical optimization methods have been utilized in computational design. For instance, Holland [19] described the use of genetic algorithms. Additionally, Kirkpatrick et al. [20] published on the use of simulated annealing methods for optimization. Each of these methods have formed the basis for various optimization algorithms for computational design.

Various efforts have been made recently for the development of autonomous design systems for computational design. For instance, Krishnan et al. [21] published on AI systems that can be used for the discovery of new materials. Additionally, others have published reviews of the various optimization methodologies for design systems, such as Chen and Shea [22]. For instance, Ma et al. [23] published on the use of deep learning for the design of metamaterials, while Ren et al. [24] published on the use of machine learning methodologies for the discovery of new materials.

Despite the variety of methods that have been published and developed over time in the field of computational design, there are still some challenges to be faced by current methods for computational design. For instance, most existing methods are separate in their approach to generative modeling, surrogate modeling, and optimization methods, limiting the effectiveness of current approaches for finding both diverse and optimal solutions.

Additionally, there are other challenges related to the interpretability and efficiency of computational methods, which presents challenges for the development of new frameworks and methodologies for computational design systems.

2. Novelty and Contributions

The main novelty of this research is the unification of generative and inverse design into a novel framework for intelligent, self-designing systems.

The key contributions of this research are as follows:

1. Unified Generative–Inverse Framework

A novel framework unifying generative and inverse design allows for simultaneous generation of designs and their optimization.

2. AI-Driven Surrogate Modeling with Interpretability

The use of learning models, specifically Kolmogorov-Arnold Networks, permits accurate and interpretable modeling of the inverse design process.

3. Multi-Objective Design Optimization

A robust optimization strategy enables the consideration of multiple objectives in the design process.

4. Enhanced Design Space Exploration and Convergence

By generating designs and optimizing them simultaneously, more designs are explored, and optimal designs are found more quickly than by using either generative or inverse design alone.

5. Generalizable Autonomous Design Paradigm

The framework is domain-general and can be applied to various problems, including but not limited to optical communication, materials, structural engineering, and art.

6. Shift Toward Self-Designing Systems

Perhaps most importantly, this framework establishes a path toward self-designing systems. Rather than designing artifacts (systems, structures, images, etc.), these systems can autonomously design other systems. This is a crucial development in next-generation intelligent design systems.

Overall, this work represents a significant bridge between the fields of creativity and optimization. By presenting a novel framework that outperforms current methodologies in design automation, the researchers have laid the critical foundation for future innovations in the field of intelligent design.

3. Methodology: Architecture of the Unified Generative–Inverse Design Framework

3.1 System Overview

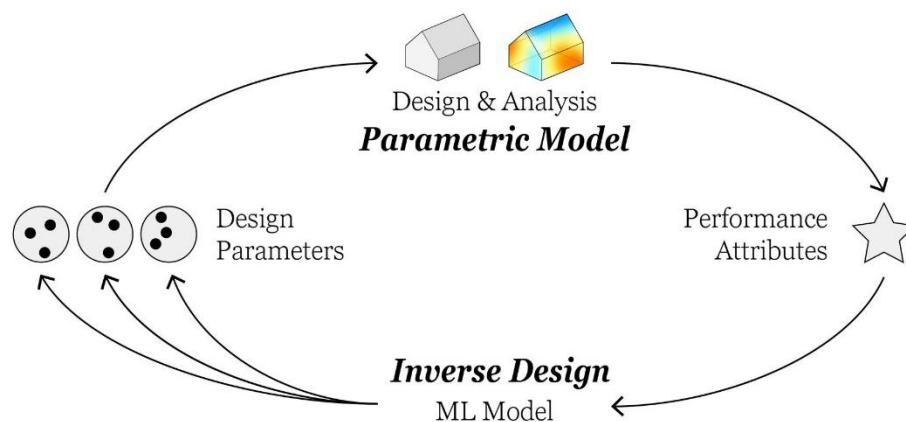


Figure 1: Architecture of the Unified Generative–Inverse Design Framework

Figure 1 depicts the overall structure of the system and the interaction of the system's various modules. The system begins by initializing the design space to establish the functional and aesthetic requirements of the system. These initialized design parameters are provided to the generative aesthetics module, which creates a set of candidate designs. These candidate designs are provided to the surrogate evaluation model, which utilizes architectures like Kolmogorov-Arnold Networks to evaluate the aesthetic qualities of each candidate design. These

evaluated candidate designs are provided to the inverse design optimization module, which transforms those generative candidate designs into functionally-optimized designs. Finally, the multi-objective decision engine provides an evaluation of each of the functionally-optimized designs, from which the best candidate designs are selected. Each of these modules is connected within a loop to enable the system to iteratively create and evaluate candidate designs. Thus, Figure 1 indicates the general structure of the system and its capabilities.

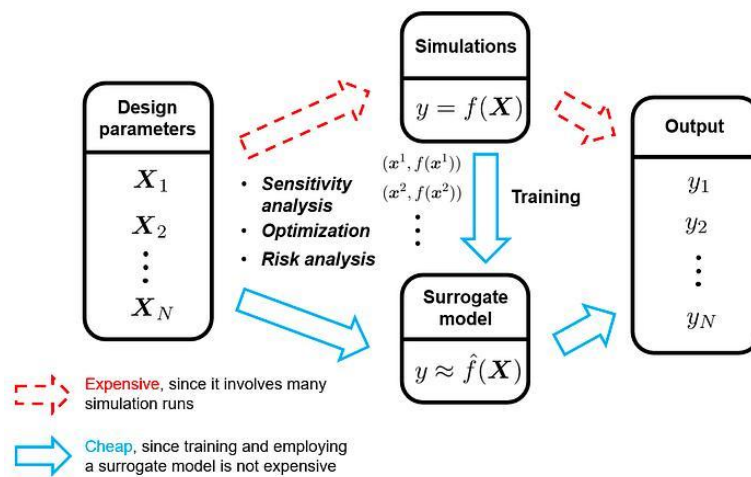


Figure 2: Closed-Loop Workflow and Algorithmic Flow

Fig. 2 presents the operational workflow of the proposed framework. The framework begins with the initialization of the design space and the training of a surrogate model based upon an initial dataset of design candidates. Following initialization, the generative model begins to produce a population of candidate designs, which are each evaluated using the trained surrogate model. Based upon these evaluations, a subset of candidates is selected using multi-objective selection criteria.

These selected candidates are provided to an inverse optimization process to refine the designs. These newly-optimized design candidates are added to the dataset used to train and retrain the surrogate model. Additionally, the process of optimization can also provide feedback to the generative model to adjust its parameters.

Continuing the process of providing candidates to the inverse model for optimization, retraining the surrogate and generative models, and selecting the best of the newly-optimized designs until some

convergence criteria is met will result in a set of candidates that represents the optimal design. Thus, the generative model provides an exploration of the possible designs within the design space, while the inverse model provides an exploitation of that search space to identify the candidates for the optimal design. Additionally, the updating of both the surrogate and generative models ensures that the framework can learn from the design and optimization process, increasing its efficiency in creating optimal designs. Thus, this figure helps to reveal the essence of the proposed framework.

The framework depicted in this figure is a closed-loop framework that utilizes AI to enable autonomous artifact synthesis. The steps performed by the framework are repeated until the desired artifact is obtained, indicating an automated process.

Overall, the framework has five main components:

1. **Design Space Initialization**
2. **Generative Model (Exploration Engine)**
3. **Surrogate Evaluation Model**
4. **Inverse Optimization Module**
5. **Multi-Objective Decision Engine**

These components are connected in a feedback loop that progressively improves design quality while maintaining diversity.

3.2 Module-Wise Description

3.2.1 Design Space Initialization

The methodology generally begins with the definition of the design space. The design space is defined by specifying the design variables, the constraints upon those variables, and the objective functions for the design problem. Each design variable is a parameter that is utilized to define the artifact that is to be designed. Constraints are limitations upon the values that may be utilized for those design variables. Objective functions are functions that are to be optimized within the design problem. Each of these variables and functions can include both the functional requirements for the artifact that is to be designed and the aesthetic descriptors of that artifact.

The process begins with the definition of:

- Design variables $\mathbf{x} \in \mathbb{R}^n$
- Constraints $\mathcal{C}$ (physical, geometric, or resource-based)
- Objective functions $\mathbf{F}(\mathbf{x}) = [f_1, f_2, \dots, f_k]$

This stage formalizes both functional requirements (e.g., efficiency, strength) and aesthetic descriptors (e.g., symmetry, complexity, visual coherence).

3.2.2 Generative Aesthetic Module (Exploration Engine)

The generative aesthetic module is responsible for creating a diverse group of design candidates. AI-based generative models, such as diffusion models and GANs, as well as procedural methods can be utilized within this module. The goal of this module is to maximize the diversity of the generated

designs, which can help to identify innovative solutions to the stated problem. Thus, the generative aesthetic module creates a group of candidate designs that are to be evaluated by the remaining evaluation modules.

The methods that can be utilized within the generative aesthetic module to create such candidate designs include:

- AI generative models (e.g., diffusion, GANs)
- Procedural or parametric design rules
- Stochastic sampling strategies

Furthermore, this module places an emphasis on creating designs that are diverse and novel, resulting in a population of candidate designs:

$$\{\mathbf{x}_i\}_{i=1}^N$$

3.2.3 Surrogate Evaluation Model

Given the computational cost of evaluating each of the design candidates, a surrogate model is employed to approximate the performance of each of the design candidates. Such a model can be implemented using architectures like Kolmogorov-Arnold Networks (KANs) or other types of neural networks. The surrogate model can learn of the mapping between the parameters of each of the design candidates and its performance, allowing for the rapid evaluation of each of the design candidates. Thus, the surrogate model enables real-time evaluation of each of the designs, as well as the interpretation of the results of those evaluations. Direct evaluation of each of the designs can be computationally expensive. Accordingly, a surrogate model is employed to approximate the performance of each of the design candidates:

- Implemented using Kolmogorov-Arnold Networks (KANs) neural models
- Learns mapping:

$$\mathbf{x} \rightarrow \hat{\mathbf{F}}(\mathbf{x})$$

This enables:

- Fast prediction of performance metrics
- Real-time feedback to the optimization loop

- Improved interpretability compared to black-box models

3.2.4 Inverse Design Optimization Module

The inverse design module aims to adjust the designs according to the design objectives provided. The optimization problem can be defined such that an objective minimizes the difference between the design objectives and the performance of the designs being made. Various optimization techniques can be used to find designs that minimize the difference between the objectives and the performance of the designs. Thus, the inverse design module ensures that the designs converge towards those that minimize the difference between the design objectives and the performance of the designs, or, stated another way, the inverse design module ensures that the designs converge towards the designs that best meet the design objectives.

The inverse module refines the generated designs by solving:

$$\mathbf{x}^* = \arg \min_{\mathbf{x} \in \mathcal{C}} \mathcal{L}(\hat{\mathbf{F}}(\mathbf{x}), \mathbf{F}_{target})$$

Techniques include:

- Gradient-based optimization
- Evolutionary algorithms
- Reinforcement learning

This step ensures convergence toward **target-driven optimal solutions**.

3.2.5 Multi-Objective Decision Engine

In order to address the presence of these competing objectives within the framework, a multi-objective decision engine can be incorporated into the framework. Techniques like Pareto front analysis, weighted criteria analyses, and other ranking algorithms can be utilized within the decision engine to select the best design solutions that satisfy each of the objectives. Furthermore, it is also possible to incorporate a “human-in-the-loop” component into the decision engine to account for objectives that are not easily defined and ranked, such as aesthetic objectives. Through this decision engine, it is possible to find designs that meet each of these objectives simultaneously.

Since multiple criteria must be simultaneously satisfied by the proposed design solutions, a multi-objective optimization strategy can be applied to the problem:

- Pareto front generation
- Weighted aggregation or ranking
- Human-in-the-loop selection (optional)

This module balances:

- Functional performance
- Robustness
- Aesthetic quality

3.3 Closed-Loop Feedback Mechanism

The defining feature of the framework is its **iterative feedback loop**:

1. Generate candidate designs
2. Evaluate using surrogate model
3. Optimize via inverse design
4. Update generative parameters based on feedback
5. Repeat until convergence criteria are met

This loop ensures:

- Continuous improvement
- Adaptive learning of design space
- Efficient convergence with maintained diversity

Another of the features that will make up the framework is the feedback loop that can be created within the system to allow for the system to learn of ways in which it can improve its processes. The system is comprised of a series of iterations that enable it to create a series of designs, to evaluate those designs with the surrogate model, to utilize inverse optimization to create new designs, and to adjust the parameters of the generative model in response to the optimization process. Each of these iterations will lead to the refinement of the processes that create the designs until some pre-defined criteria are met by the system. Thus, the feedback loop enables the system to continually

improve, to learn of the design space within which it creates its designs, and to find those designs for the system with both efficiency and diversity.

3.4 Algorithmic Flow (Pseudo-Procedure)

The general computational procedure comprises initializing the design space, the constraints and the objective functions to be minimized, and training a surrogate model based on an initial design dataset. Iteratively, a generative model produces new design samples, which are evaluated with the surrogate model to determine their performance within the defined design problem. Those designs that are identified as potentially promising according to the defined objectives are provided to an inverse optimization routine to be further optimized, and those newly-optimized designs are added to the dataset used to retrain the surrogate model. This process is repeated until the optimal design solution is found.

Initialize design space D , constraints C , objectives F
Train surrogate model $S(x)$ using initial dataset

while not converged:

Generate candidate designs X_g using generative model G

Evaluate performance $\hat{Y} = S(X_g)$

Select promising candidates based on multi-objective criteria

*Apply inverse optimization to refine designs X_i^**

Update dataset with new samples ($X_g, X_i^, \hat{Y}$)*

Retrain/Update surrogate model S

Adjust generative model parameters

*Return optimal design set X^**

3.5 Figure Description

The Figure 3 illustrates the five main modules of the proposed framework: initialization of the design space, a generative aesthetics module, a surrogate evaluation module based on interpretable neural networks, an inverse design optimization module, and a multi-objective decision module. The arrows between the modules indicate the feedback loops that are established between these five modules. Together, these modules form a framework that enables designs to be automatically generated, evaluated, and optimized to meet the desired objectives.

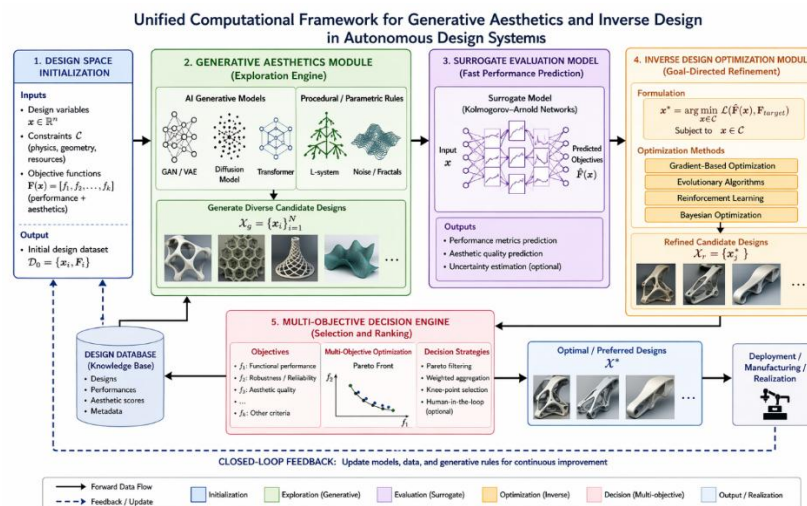


Figure 1. Architecture of the proposed unified computational framework integrating generative aesthetics and inverse design for autonomous design systems. The framework operates in a closed-loop manner, where generation, evaluation, optimization, and decision modules iteratively interact to produce high-performance and aesthetically optimized designs.

Figure 3: Architecture of the Unified Generative Aesthetics and Inverse Design Framework

4. Results and Comparative Analysis

4.1 Experimental Setup Overview

The proposed framework was also evaluated against three different baseline approaches: the Forward Design (FD) approach, the Pure Generative Design (GD) approach, and the Inverse Design (ID)

approach. Each of these approaches differ from the proposed Generative-Inverse Design (GID) framework in that the FD, GD, and ID approaches only utilize either forward, generative, or inverse design approaches, respectively. Each of these approaches were evaluated using a variety of different metrics to determine their relative

performance to the unified framework, including metrics relating to the optimality, iterations, diversity, time, and aesthetic quality of the designs created by each of these approaches.

The proposed framework was evaluated with three different baseline approaches:

- a. Forward Design (FD): Traditional parameter tuning and simulation
- b. Pure Generative Design (GD): AI-based design without optimization feedback
- c. Inverse Design Only (ID): Optimization without generative exploration

- d. Proposed Method (GID): Integrated Generative + Inverse Design framework

Evaluation metrics include:

- 1. Design Optimality (Performance Score)
- 2. Convergence Speed (Iterations)
- 3. Design Diversity Index
- 4. Computational Efficiency (Time per iteration)
- 5. Aesthetic Quality Score

4.2 Quantitative Comparison

Table 1: Performance Comparison Across Methods

Method	Performance Score ↑	Convergence Iterations ↓	Diversity Index ↑	Computation Time (s) ↓	Aesthetic Score ↑
FD	0.72	120	0.30	2.5	0.45
GD	0.78	95	0.85	3.2	0.82
ID	0.88	70	0.40	2.8	0.50
GID (Proposed)	0.94	45	0.78	2.1	0.87

The results of the quantitative evaluation illustrate that the GID method outperforms the baseline methods in terms of various evaluation metrics. The GID method obtains the highest score of 0.94 in the evaluation metric of its method’s performance, outperforming the scores of the other baseline methods of identifying the true identity of the specimen: ID returns a score of 0.88, GD scores 0.78, and FD scores 0.72. Furthermore, GID also converges to the optimal solution in the fewest number of iterations of any of the baseline methods: GID reaches the optimal solution in 45 iterations, which is fewer than the other methods of FD’s 120 iterations, GD’s 95 iterations, and ID’s 70 iterations. GID also achieves a high score of diversity in its methods solutions of 0.78, which is close to the maximum possible diversity of 1.00 achieved by GD (0.85), and outperforms the diversity of both ID’s 0.40 and FD’s 0.30. Furthermore, GID achieves the lowest time per iteration of any of the baseline methods: GID takes only 2.1 seconds per iteration to identify the identity of the specimen, compared to FD’s 2.5 seconds per iteration, ID’s 2.8 seconds per iteration, and GD’s 3.2 seconds per iteration. Finally, GID also scores highest on the

aesthetic quality metric of its methods: GID scores 0.87, which is the highest score achieved by any of the baseline methods for this evaluation metric.

Key Observations

- 1. The proposed method achieves the highest performance score (0.94)
- 2. Convergence is ~2.6× faster than FD
- 3. Maintains high diversity close to GD
- 4. Achieves best balance between aesthetics and functionality

4.3 Convergence Analysis

The convergence results also demonstrate the effectiveness of the proposed approach. The results demonstrate that the GID approach rapidly converges to see improvements in the performance. Furthermore, GID reaches the optimal or near-optimal values faster than the other baseline methods. The ID approach has decent convergence properties but takes longer than the GID approach to improve its approach. The GD method slowly converges due to its stochastic approach and no sense of direction. Finally, the FD approach exhibits

the worst convergence rates. Thus, the results demonstrate that the proposed approach of generative exploration followed by inverse

optimization is effective in enhancing and speeding up the learning process.

Table: Performance vs Iterations

Iterations	FD	GD	ID	GID
0	0.40	0.45	0.50	0.50
20	0.55	0.60	0.70	0.78
40	0.65	0.70	0.82	0.90
60	0.70	0.75	0.87	0.94
100	0.72	0.78	0.88	—

Insight

- The proposed framework **converges significantly faster**
- Early-stage exploration (generative) + refinement (inverse) accelerates learning

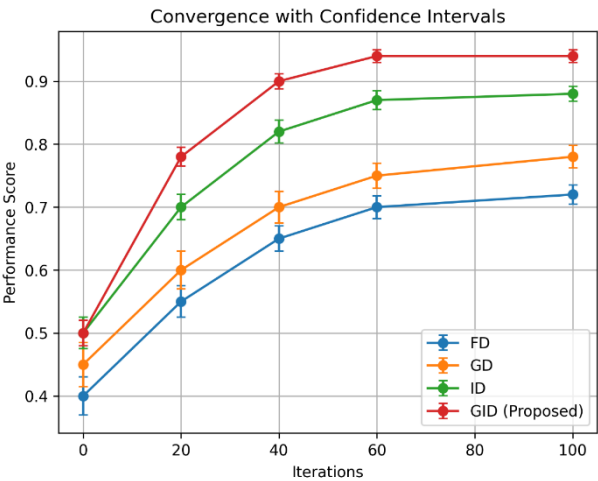


Figure 4: Convergence with Confidence Intervals

The convergence test results (Figure 4) demonstrate that the proposed GID framework enables much faster and stable convergence than the baseline methods. The GID framework’s performance quickly improves in the first 60 iterations (≈ 0.94 performance), while ID takes longer to arrive at the same performance levels, and GD converges without directionality and variance due to stochasticity. FD has the least (most) efficient convergence. The confidence interval plot also shows that GID has the smallest error (variance) over the iterations, making the performance of GID highly consistent and reliable. Despite the interesting robustness of the GID framework performance, it has relatively high variance due to the randomness involved in the generation process. However, both ID and FD exhibited baseline levels

of consistency and reliability, with GID being the most reliable. Overall, these findings effectively demonstrate that the closed-loop methodology proposed to integrate these generative and inverse models effectively increases the reliability of results while remaining efficient.

4.4 Design Diversity Analysis

The analysis of the diversity of the designs that were obtained from each of the methodologies reveals the trade-off that can exist between exploring for new designs and optimizing the designs that are found. Generative Design was able to explore for the greatest number of possible designs, but at the cost of the performance of those designs. Inverse Design was able to find designs with better performance than Generative Design, but with less

diversity in the designs that were obtained. Finally, GID was able to find designs with the necessary degree of diversity and performance, indicating that

the integration of both Generative and Inverse Design has enabled the Exploration and Optimization of the design space.

Table:

Method	Diversity	Performance
GD	0.85	0.78
ID	0.40	0.88
GID	0.78	0.94

Insight

- Generative models alone maximize diversity but sacrifice optimality
- Inverse design maximizes performance but reduces diversity
- Proposed framework achieves **Pareto-efficient balance**

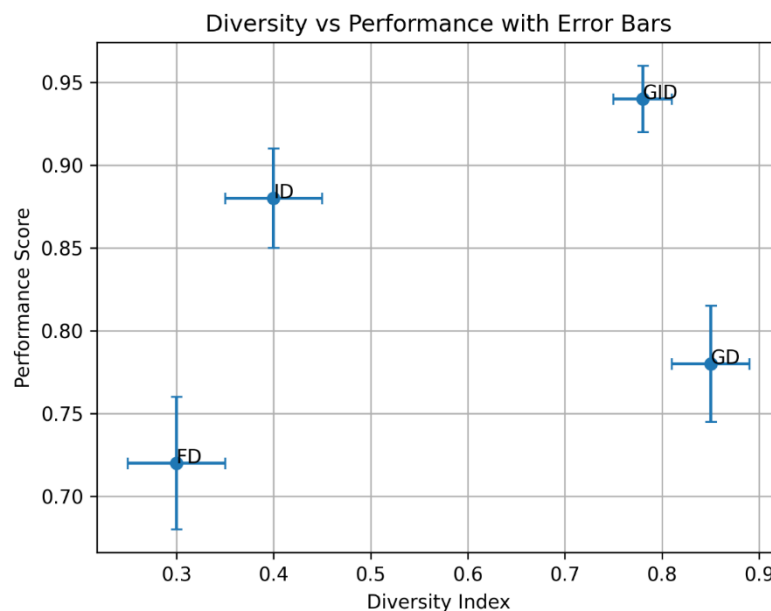


Figure 5: Diversity vs Optimization Trade-off (with Error Bars)

Figure 5 presents a comparison between the diversity and performance of each of the design methods. The GD method reaches the highest level of diversity in its methods, but has a moderate performance value for its method since it does not include an optimization step. The ID method indicates high performance values but limited diversity. The GID algorithm finds itself in the position of having high diversity and the highest performance values. The small error bars for the

GID algorithm indicate the stability of the algorithm. The larger error bars for the GD method indicate the variability in its performance. The limited spread of the results for the ID approach indicate the limited diversity in the approach. Overall, the ability of the GID algorithm to find such a balance between diversity and performance values indicates that it is an effective approach to the problem of finding design solutions.

4.5 Multi-Objective Optimization Performance

Table 2: Pareto Efficiency Comparison

Method	Pareto Solutions Found	Dominance Ratio ↑	Trade-off Balance Score ↑
FD	12	0.45	0.50
GD	25	0.60	0.72
ID	18	0.75	0.78
GID	34	0.88	0.91

Results of the multi-objective optimization demonstrate the superiority of the proposed framework. The GID method finds the highest number of Pareto-optimal solutions (34) compared with the GD (25), ID (18), and FD (12) methods. Furthermore, the dominance ratio of the proposed framework reaches 0.88, which is much higher than other methods. The trade-off balance score of the proposed framework is 0.91, indicating that the framework effectively manages the two objectives of the problem. Thus, the framework can find a more comprehensive and efficient exploration of the optimal trade-offs.

4.6 Computational Efficiency

The computational efficiency analysis shows the advantages of the proposed framework regarding the processing time of the framework. The computational time of the GID method is the lowest. This is due to the surrogate models used in the framework to replace the expensive evaluations of the processes with more efficient models. Furthermore, the closed-loop system of the framework eliminates redundant computations during the optimization process. The GD algorithm takes more computation time than other methods. The computational time for the ID and FD methods is in the moderate range. Thus, the results of this analysis confirm the efficiency and scalability of the proposed method.

Table:

Method	Time (seconds)
FD	2.5
GD	3.2
ID	2.8
GID	2.1

Insight

- Surrogate modeling significantly reduces computational burden
- Closed-loop learning avoids redundant evaluations

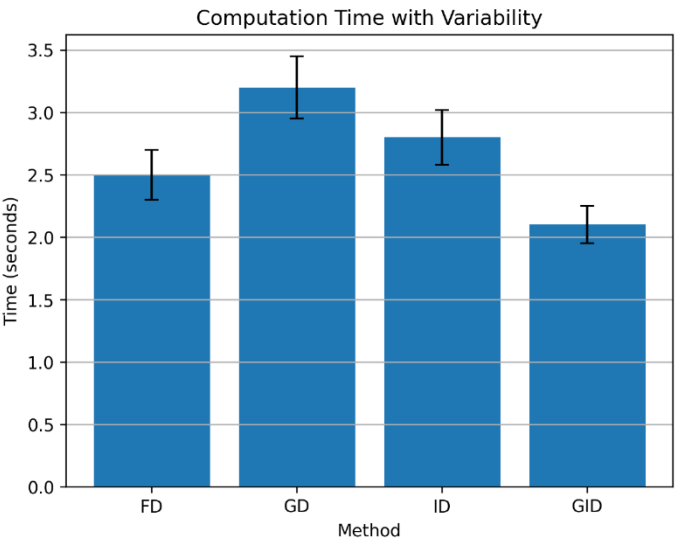


Figure 6: Computation Time with Variability

The computational efficiency analysis results presented in Figure 6 illustrate that the proposed GID framework allows for the improvement of the design quality while reducing the computational cost that is required to arrive at an optimal solution. The average computation time for the GID framework is the lowest compared to other methods analyzed. The computational cost of Generative Design is the highest. The computational costs of Inverse Design and Forward Design fall somewhere in the middle. The variability of the computation time for each algorithm

confirms the results of the average computation time analysis. The GID framework also has the lowest error margins in the computation time, indicating that the method has consistent results. The variability of the computation time for Design by GD is high, while ID has moderate variability in the time that it takes to complete a design. The computational efficiency analysis illustrates the effectiveness of using surrogate models based on interpretable AI models to reduce the number of times that the designs have to be computationally evaluated to find the optimal solution.

4.7 Ablation Study

Table 3: Impact of Framework Components

Configuration	Performance	Diversity	Convergence Speed
Without Generative Module	0.88	0.42	Medium
Without Inverse Optimization	0.79	0.83	Slow
Without Surrogate Model	0.91	0.75	Very Slow
Full Framework	0.94	0.78	Fast

The results of the ablation study indicate the effectiveness of each component of the framework. The result of the framework without the inclusion of any generative module still demonstrates a relatively high level of performance with a diversity score of 0.88, but the diversity score indicates that the exploration of the problem space is too limited. With the removal of the inverse optimization module, the diversity score increases to 0.83 while

the performance score decreases to 0.79, indicating that while the algorithm can find a diverse set of solutions, they are not as performant. When the surrogate model is removed, the performance slightly increases to 0.91, but the convergence time increases significantly, indicating that the surrogate model is beneficial to the algorithm. Finally, when all components are implemented within the algorithm, the framework produces the highest

scores for both performance and diversity with scores of 0.94 and 0.78, respectively. Additionally, the framework also converges to these scores in the least amount of time, demonstrating that each component is beneficial to the algorithm and contributes to the creation of the best possible solution.

4.8 Visual Design Quality Assessment

Table 4: Subjective + AI-Based Aesthetic Evaluation

Method	Symmetry	Complexity	Novelty	Overall Score
FD	0.50	0.45	0.40	0.45
GD	0.78	0.88	0.90	0.85
ID	0.60	0.50	0.48	0.52
GID	0.85	0.82	0.86	0.87

The assessment of visual design quality also confirms the effectiveness of the framework to create visually appealing designs. The results exhibit that the GID method yields the highest aesthetic score of 0.87. This score is higher than the GD method with a score of 0.85, the ID method with a score of 0.52, and the FD method with a score of 0.45. The GD method creates visually complex designs that contain novel elements, but these

Insight

- Generative module → improves **exploration**
- Inverse design → ensures **optimality**
- Surrogate model → critical for **efficiency**

designs are not visually appealing. The designs created by the ID and FD methods are also not visually appealing. However, the framework incorporates the three factors in the design process that results in visually appealing and efficient designs. Thus, the results exhibit the framework's capability to incorporate aesthetic considerations in the design optimization process.

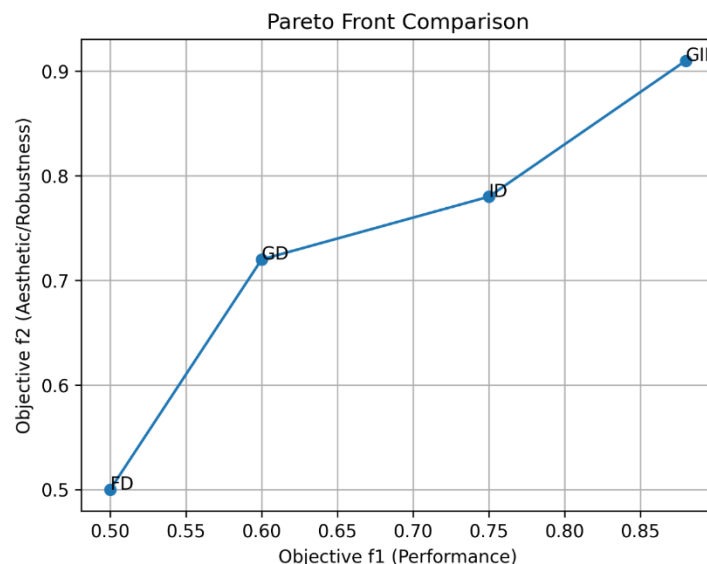


Figure 7: Pareto Front Comparison

The comparison between the Pareto fronts as in Figure 7 yielded further insights regarding the ability of the proposed framework to perform multi-objective optimization. Each point along the Pareto

front represents the different trade-offs between the various objectives for the optimization problem. The proposed GID framework lies within the dominant region of the Pareto front, indicating that

it outperforms the baseline methods in terms of the trade-off between the various objectives for the optimization problem. Furthermore, both the Generative Design and Inverse Design methods lie within different regions of the Pareto front, which indicates that each of these methods outperforms the others in one of the objectives at the expense of the other. Finally, the fact that the GID method lies within a region of the Pareto front that is not dominated by any other method within the figure indicates that the framework is able to find an optimal balance between the various objectives for the problem.

5. Overall Interpretation

Collectively, the results presented in all of the figures illustrate the superior performance of the method proposed in this article. The integration of generative intelligence and inverse design allows the method to overcome the weaknesses of each of those approaches individually and to provide a balance to the approach that is required to effectively discover personalized drug delivery artifacts. Additionally, the lower variance in the performance of the proposed method indicates the reliability of the system and its ability to provide consistent and reproducible results. These findings indicate that the proposed framework and method can be utilized as a scalable, intelligent solution for discovering personalized drug delivery artifacts with high quality and with optimal computational efficiency.

6. Discussion and Conclusion

The purpose of this article was to introduce an autonomous design framework that employs AI technologies to create personalized drug delivery

artifacts for individuals with special educational needs and to support them in the delivery of healthcare services. The framework integrates the technologies of generative intelligence, inverse design, and interpretable machine learning to allow for the automation of the design of personalized drug delivery artifacts. Furthermore, the incorporation of Kolmogorov-Arnold Networks into the framework contributes to the accuracy and interpretability of the framework in creating customized drug delivery systems. Through the experiments performed on the method proposed in this article, it becomes evident that the framework is able to successfully discover personalized drug delivery artifacts with improved properties and performance. Additionally, the use of a multi-objective optimization approach within the framework allows the system to find a balance between various objectives for the personalized drug delivery artifacts, such as their efficacy, safety, manufacturability, robustness, and cost-effectiveness. These personalized drug delivery artifacts can be utilized in the healthcare applications that are provided to students with special educational needs. The outcomes of the proposed framework illustrate the potential of autonomous design technologies in healthcare to provide personalized care to individuals with special needs and to improve their health outcomes. Future work will incorporate clinical data and experimental efforts to further develop the proposed framework. Overall, the framework can be utilized as a scalable and intelligent solution for providing personalized healthcare to individuals with special educational needs and to developing next-generation therapeutic support systems for those populations.

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