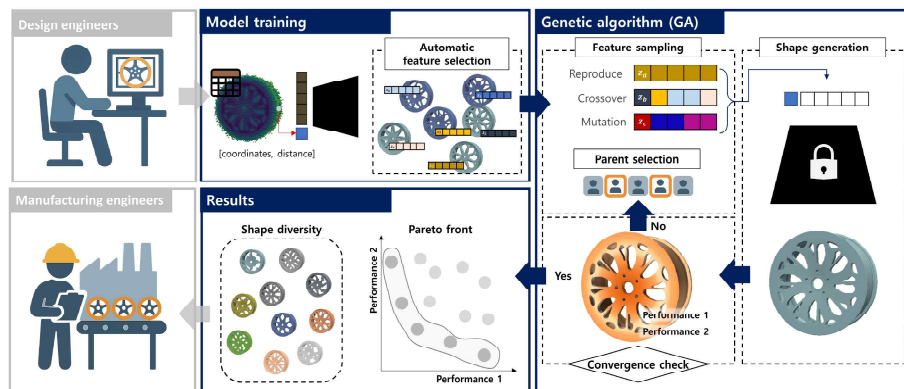


Graphical Abstract

Three-dimensional Deep Shape Optimization with a Limited Dataset

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Highlights

Three-dimensional Deep Shape Optimization with a Limited Dataset

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Overcomes explicit parameterization limits using data-driven shape optimization

Optimizes 3D shapes effectively with a limited dataset approach.

Achieves diverse design outcomes in multi-objective optimization

Validates the advanced performance of the framework through multiple experiments

Three-dimensional Deep Shape Optimization with a Limited Dataset

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Abstract

Generative models have attracted considerable attention for their ability to produce novel shapes. However, their application in mechanical design remains constrained due to the limited size and variability of available datasets. This study proposes a deep learning-based optimization framework specifically tailored for shape optimization with limited datasets, leveraging positional encoding and a Lipschitz regularization term to robustly learn geometric characteristics and maintain a meaningful latent space. Through extensive experiments, the proposed approach demonstrates robustness, generalizability, and effectiveness in addressing typical limitations of conventional optimization frameworks. The validity of the methodology is confirmed through multi-objective shape optimization experiments conducted on diverse three-dimensional datasets, including wheels and cars, highlighting the model's versatility in producing practical and high-quality design outcomes even under data-constrained conditions.

Keywords: Signed Distance Function, Artificial Intelligence, Limited Dataset, implicit neural representation, Shape Optimization

Introduction

Artificial intelligence (AI) has shown significant achievements in various domains, including regression, classification and segmentation [1, 2]. Building upon these advancements, research in mechanical design, such as computer-

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aided design (CAD) and computer-aided engineering has increasingly utilized AI to overcome the limitations of traditional methodologies and provide new insights.

Deep generative models (DGMs) such as the variational autoencoder (VAE), the generative adversarial network (GAN) and the diffusion model, have garnered increasing attention due to their ability to learn from data and create new data that were not previously accessible [12, 13, 14]. This characteristic is a significant solution to the persistent data scarcity problem in the mechanical domain unlike conventional generative design approaches. DGMs guarantee data diversity facilitating the generation of design suggestions that incorporate engineering functionality.

Traditional parametric shape optimization produces different optimal results depending on how feature selection is performed. This difference becomes more pronounced for complex shapes with highly dependent parameters. In contrast, AI models can automatically analyze the feature set data through learning and compress data into a latent space. From an optimal design perspective, the latent space can be used as design variables providing automatic feature selection functionality.

One of the significant issues in employing DGM for mechanical design lies in the need for varied data within the same category. Mechanical parts, which are fundamentally mass-produced, do not have abundant data within the same design domain and existing data show only minimal variation. These intrinsic data characteristics create significant challenges for AI when attempting to identify subtle distinctions within a single category as it tends to focus on the overall form, which can lead to issues like mode collapse.

This study aims to propose a three-dimensional (3D) deep learning model tailored for optimal design applications. The proposed model automatically selects features from generative AI training data while preserving shape diversity. Furthermore, the proposed model demonstrated robust performance on limited datasets, addressing a bottleneck previously identified in optimal design approaches. This research introduces a versatile shape optimization framework using AI models. This study investigates shape optimization across distinct datasets, an endeavor that conventional parametric techniques and existing DGM-based approaches have yet to achieve. In addition, this framework is applied to shape optimization problems demonstrating its universality through optimizations performed via computational fluid dynamics (CFD) and finite element method (FEM) simulations.

This paper is structured as follows. Section 1 introduces previous research

on shape optimization, topological optimization and shape optimization using DG and discusses data representation and deep learning architecture in the context of D data. Section provides an overview of the entire framework of this study from data collection to shape optimization. Section examines the originality and validity of the methodology through three shape optimization experiments. Finally, Section presents conclusions and directions for future work.

Related works

Shape Optimization method

Parametric Shape Optimization

Data generated through CAD programs consists of combinations of various geometric variables which can be utilized as design parameters in the optimization process. Parametric shape optimization is a design method in which design parameters, within a predefined range, satisfy constraints based on a defined CAD model while simultaneously identifying the optimal shape to minimize the objective function. This method is widely used in various engineering fields, including automotive, aerospace, electromagnetic and acoustic.

Parametric shape optimization has advanced with surrogate modeling for predicting engineering performance because it allows for defining data within a specified range via design parameters. In particular, substantial progress has been made in areas where the data can be easily defined by simple curves or encapsulated by numerical characteristics. Experimental results indicate that the extensive design space and intricate parameter dependencies enable heuristic optimization methods such as the non-dominated Sorting Genetic Algorithm (NSGA-II) to outperform gradient-based approaches.

For non-parametric data such as D meshes, parameterization can be performed using techniques like polynomial mapping or free-form deformation. These methods can be implemented relatively easily and transform complex and detailed shapes. Furthermore, when constructing surrogate models, mesh data can be represented as a graph and processed with graph neural networks, enabling the solution of more generalized problems. However, a limitation of these methods is that, depending on the resolution of the defined parameters, capturing fine details becomes challenging and the number of parameters increases.

Topology Optimization-based Generative Design

Topology optimization is the most effective method for generating shapes that satisfy prescribed boundary conditions and meet specific objective functions.

This methodology has undergone numerous advancements since introducing the initial solid isotropic material with penalization approach in the academic literature.

It is the most widely utilized method in the field of generative design because it can generate new data based on constraints defined by designers.

In generative design, topology optimization explores new shapes throughout the design process, from problem definition to detailed design. This approach streamlines the process by numerically evaluating and generating optimal designs, producing better outcomes than traditional stage-by-stage methods.

Generative models that leverage topology optimization excel in data generation under multiple boundary conditions, allowing the production of various designs. However, a notable drawback is that they tend to yield many similar data instances.

To overcome these limitations, recent studies have increasingly focused on combining topology optimization with deep generative models. For example, Oh et al. used topology optimization to create seed data to train a deep generative model.

They then trained a GAN model to generate diverse wheel designs with various spoke configurations.

Furthermore, there are emerging cases that incorporate reinforcement learning to address design diversity and multi-objective requirements.

Deep Generative Model-based Shape Optimization

Recent research on deep generative models has been advancing significantly. Intensive work is being carried out on creating generative models such as GANs, VAEs and diffusion models, which are capable of generating new images and shapes.

Deep generative models have evolved according to the type of data involved. For instance, they are particularly effective for processing non-parametric data such as images or 3D meshes and extracting low-dimensional features. In the field of optimal design, research is being conducted on generating and optimizing shapes using deep generative models.

Optimization studies utilizing DGMs have seen significant advancements in domains that are well-suited for image representation, such as meta-structures or airfoils, which are relatively easy to parameterize.

In particular, new architectures have been developed to better define air-

foils, typically represented by Bézier curves, to improve the feasibility of the generated data

or D data architectures based on implicit neural representations as introduced by Bar et al. have been widely adopted. These models are highly versatile serving not only as generative models but also as surrogate models. Their ability to perform auto-differentiation makes sensitivity analysis straightforward making them well-suited for capturing local variations. This approach has been particularly useful for vehicle aerodynamic optimization problems which typically require high computational resources.

Overall data-driven deep generative models distinguish themselves from topology optimization-based generative design in that they can explore more realistic data distributions and discover unique configurations. However, they require large amounts of data.

	Topology Optimization	Parametric Shape Optimization	DG-based Shape Optimization	Proposed Method
Parameterization	Automatic	Manual	Automatic	Automatic
Interpolation	Flexible	Flexible	Possible	Possible
Convergent possibility	Bad	Good	Good	Good
Training data	One	One	Large	Small minimum

Table Comparison with other optimization methods

In summary, Section 4.1 is concisely represented by Table 4. Although DG-based shape optimization successfully addresses the limitations of traditional topology optimization and parametric shape optimization methods, it still suffers from a critical drawback: requiring an extensive training dataset. This study addresses this issue by proposing a robust model that delivers strong performance even with limited datasets, making it particularly suitable for shape optimization applications. Detailed descriptions and explanations are provided in Section 4.2.

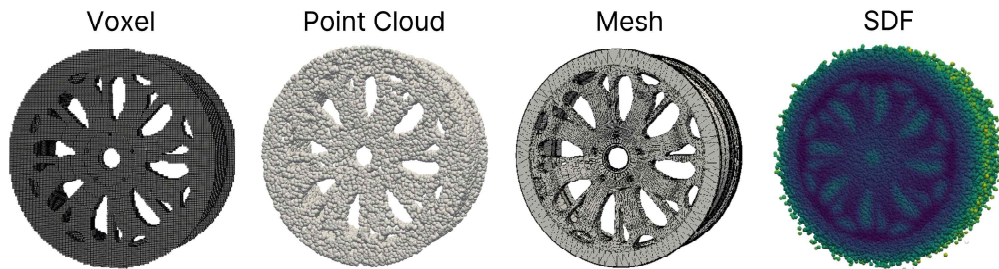


Figure 1: Four common 3D data representations

Deep Learning for 3D Data

3D Data Representation

Deep learning with 3D data representation can vary depending on the specific problem being addressed. Representation for data-driven 3D deep learning can be broadly categorized into point cloud and mesh representation as shown in Fig. 1.

First, point cloud is a representation method that discretizes 3D volume into a grid. This is advantageous because it is similar to the representation of images, making it relatively easy to apply to traditional neural networks such as convolutional neural networks. However, using the point cloud approach to represent 3D shapes can lead to memory issues. Furthermore, representing a 3D shape as a point cloud can result in relatively unnecessary areas, leading to higher computational costs. Voxel representation is heavily influenced by resolution, which can make the shapes relatively less detailed and blurry.

Point cloud is a prominent representation method among 3D representations, particularly in applications such as classification, retrieval and segmentation. It represents a 3D surface using 3D points, allowing for detailed and global shape representations. However, it has a significant drawback in that it cannot capture connectivity or topological information between individual points and cannot generate watertight meshes.

Finally, mesh is a representation method that connects vertices and edges between them to represent the surface of a 3D shape. This method allows for the representation of detailed shapes and is memory-efficient, making it a popular choice in generative models. However, changing the topology can be challenging and self-intersection issues can arise when deforming the mesh. As a result, it is not a suitable representation for mechanical design with various topological changes.

At present, these representation methods are not suitable for learning 3D shapes, which is why there is growing interest in representing data implicitly. Implicit functions involve constructing a continuous volumetric field and embedding shapes as iso-surfaces with the signed distance function (SDF) being a prominent example. This can be expressed in terms of the coordinates in space as the signed distance to the surface as shown in Figure 1. The SDF represents the shortest distance from a point to the shape's surface while indicating whether the point is inside or outside the shape based on its sign. Specifically, for points inside the shape, the distance is negative (−) or points outside it is positive, and it is zero on the surface.

$$SDF(x, y, z) = \begin{cases} -d & \text{if } (x, y, z) \text{ is inside the shape} \\ 0 & \text{if } (x, y, z) \text{ is on the surface} \\ d & \text{if } (x, y, z) \text{ is outside the shape} \end{cases}$$

The surface of a shape represented by SDF can be expressed as the iso-surface of SDF = 0, and this can be converted into a discretized surface using algorithms such as marching cubes.

Implicit neural representation

Implicit representations such as SDF enable implicit learning, where coordinates serve as inputs to an ANN model and predict the distance value corresponding to those coordinates. Since this type of learning does not rely on discretized data, this theoretically enables exporting 3D shapes with infinite resolution and handling topological changes easily. Implicit learning can densely capture important parts of actual shapes, facilitating the generation of feasible and novel shapes. Starting with DeepSDF, the first to propose representing shapes as SDFs and learning them implicitly, several models have been introduced for shape manipulation. These include D2SDF, which adds a coarse network for shape manipulation and A-SDF, which disentangles the latent space for articulated objects. All of these models feature an auto-encoder (AE) structure with an encoder.

Unlike many generative models that reduce data dimension within a bottleneck structure, these models do not have a separate encoder for data compression. Instead, the AE inputs both coordinates and latent code into the model, and back-propagation optimizes latent code within the model.

Auto-encoder (AE) models that utilize encoders such as PointNet to compress data exist. These structures create latent codes through an encoder, which has been used to handle implicit data. The work by Wang et al. proposed a methodology for extracting both global and local features from

point clouds enabling the reconstruction of large 3D scenes. The paper introduced the idea of encoding point clouds into two-dimensional planes or 2D meshes transforming structured point cloud data into structured latent space. This methodology allows for assigning different latent codes to individual points enabling learning more detailed features in shapes. The employed autoencoder decoding using skip connections in the U-Net architecture could simultaneously learn both local and global features significantly improving the accuracy of occupancy probability for each point. The derived latent vector and coordinates are then fed into an SD network to predict the distance.

Methodology

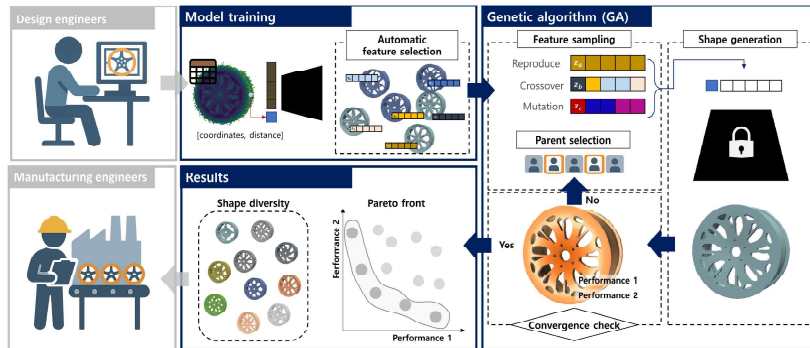


Figure 1: Overview of the proposed optimization

The overall framework of this study is illustrated in Fig. 1, which summarizes each step of the process from data collection and preprocessing to model training, feature sampling and shape generation.

Data collection

In the initial phase, a limited dataset comprising wheel and car data from both topology optimization and parametric design methods was carefully selected to demonstrate that optimization can be effective even with limited data. After preprocessing, the resulting data is validated through checks for mesh flips and watertightness [60], followed by centering, normalization and sampling surface-adjacent points with corresponding SD extraction.

Model Training: Automatic feature Selection

reprocessed data consisting of spatial coordinates and corresponding signed distances enabled the model to learn their relationships. During training, latent codes were optimized alongside the model’s weights to enhance learning. To robustly capture fine details within a limited dataset, the implicit neural representation was improved by incorporating positional encoding or high-resolution information and employing Lipschitz regularization to build a meaningful latent space. Upon training completion, the learned decoder successfully reconstructed non-parametric data and generated a latent space that effectively vectorized shape information for the extraction of geometric features.

Feature Sampling

Operator	Used
Parent selection	Tournament selection
Crossover	Simulated binary crossover
Mutation	Polynomial mutation

Table 2 Types of operators used

With the training phase complete, the decoder was frozen and feature sampling was conducted from the continuous latent space. A genetic algorithm (GA) was employed as the optimization method, wherein a population is evolved over successive generations through the operators: parent selection, simulated binary crossover, and polynomial mutation, to search for optimal solutions. Table 2 summarizes the specific operators used. In GA, individuals with higher fitness are selected as parents, combined via crossover and then undergo mutation to maintain diversity and reduce the risk of converging to suboptimal solutions. This approach is well-suited for complex optimization challenges, enabling AI-based shape optimization by refining the latent code fed into the decoder. In particular, the NSGA-2 algorithm employs crowding distance calculations to explore a broader range of solutions and uncover diverse shape designs.

Shape Generation Simulation

Using latent codes produced by the optimization algorithm, the decoder generated new shapes by producing a SD. This SD was then converted into a 3D triangular mesh using the marching cubes algorithm.

The performance of the generated shapes was evaluated via simulations. Simulations were conducted using Altair Inspire, while 3D simulations

were performed using OpenFOAM. Given the multi-objective nature of the optimization, two performance metrics with inherent trade-offs were selected: stiffness and mass for the wheel data and the drag coefficient (C_D) and lift coefficient (C_L) for the vehicle data.

Convergence check

Convergence was determined by evaluating performance metrics across a predefined maximum number of generations. If convergence wasn't achieved, the process returned to elite selection to create a new population for the next generation. Once convergence was reached, the algorithm was terminated.

Network Architecture

Mechanical design products have boundary conditions such as load and fixed conditions, resulting in minimal differences among the data. Therefore, it is important for generative models on mechanical design domains to learn the features of each dataset without significant differences between them.

Training on such a dataset with a standard multi-layer perceptron (MLP) may be problematic for two reasons. First, an MLP might fail to capture the nonlinear features of each data sample, which is critical given that many mechanical components exhibit significant performance variations due to subtle differences. Second, the limited number of available samples within the same class poses a challenge. Hence, the AutoML model must accurately learn the features of the dataset even with sparse data while developing a meaningful latent space. Positional encoding and Lipschitz regularization terms have been introduced to address these issues.

Positional encoding as outlined by Vaswani et al. and Sitzmann et al. is a powerful technique that projects input coordinates into a high-dimensional Fourier space through sinusoidal transformations as represented in

$$\gamma(p) = \begin{bmatrix} \sin(\frac{2\pi p}{L}) & \cos(\frac{2\pi p}{L}) & \sin(\frac{4\pi p}{L}) & \cos(\frac{4\pi p}{L}) & \dots & \sin(\frac{L}{2}\frac{2\pi p}{L}) & \cos(\frac{L}{2}\frac{2\pi p}{L}) \end{bmatrix}$$

p represents the input coordinates and L specifies the frequency levels in the encoding. This method allows the model to capture high-frequency information effectively before passing it to MLP.

Encoding position information across a range of frequencies, the model is able to learn various spatial features and distinguish subtle variations within the defined space. Such granularity is advantageous for learning detailed SDFs, enabling the model to capture fine details in spatially complex data.

Furthermore, these studies have confirmed that projecting inputs into a higher-dimensional space using high-resolution functions such as Fourier transformations, is highly effective for encoding complex information. This approach enhances model expressiveness and precision in capturing details.

As presented by Li et al., the Lipschitz regularization term smooths the latent space by constraining the magnitude of each layer's weight matrix. This regularization is applied to each layer's weight matrix within the L_1 as represented by the layer equation $\|eL_i\|_1 \leq b_i$

$$\|eL_i\|_1 \leq b_i \quad \text{normalization} \quad \ln \quad e^i$$

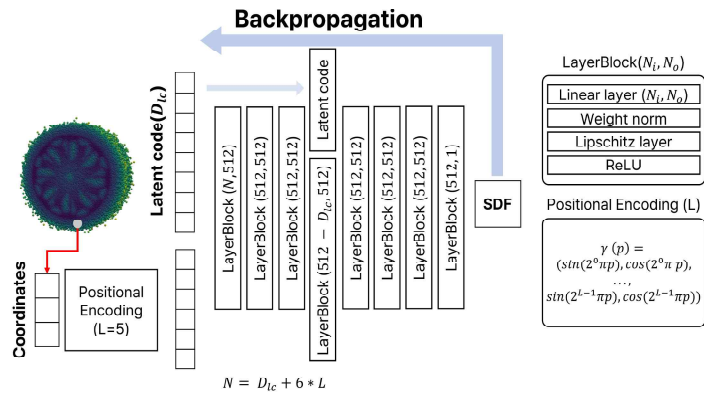
For all layers of the decoder, the Lipschitz layer normalizes the weight matrix i of each i -th linear layer using trainable Lipschitz bounds b_i as shown in

$$\text{loss}_{\text{Lipschitz}} = \sum_{i=1}^I \ln \quad e^i$$

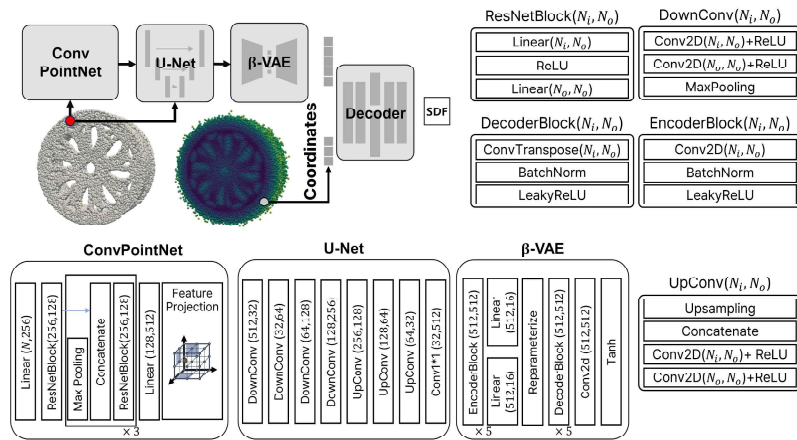
The overall Lipschitz bound for the network is determined by the product of the individual Lipschitz constants b_i assigned to each layer. As shown in a loss function, can enforce this constraint, stabilizing the model by preventing weight values from exceeding a set threshold at each layer. This regularization limits the model's response to input data, reducing excessive sensitivity and enhancing overall model stability.

This method is particularly beneficial for synthesis tasks with limited data, as it confines the model's output to a compact latent space, allowing a comprehensive representation of training data and effective pattern learning. Within the broader framework of limited-data optimization, Lipschitz regularization plays a pivotal role in fostering robust learning and ensuring reliable performance.

Two architectures were evaluated: an AD structure with an encoder and an DD structure that integrates a pointNet-based encoder ϕ , as shown in Fig. 3. This encoder inputs point cloud data π_{pcd} and extracts latent features. Both models are trained using a latent space regularization term and a truncated L_1 loss to measure discrepancies between predicted and true SDF values. The truncated L_1 loss, a modification of standard L_1 loss, truncates both positive and negative outliers to limit extreme deviations while preserving sensitivity within a specified range (δ as illustrated in Fig. 4). In experiments, δ was set to 0.05 and β was set to 0.1.



a A to decoder



b encoder-decoder

ig re model architecture

$$L_{clip} = \begin{cases} d_{pred} - d_{gt} - \delta, & d_{pred} - d_{gt} > \delta \\ d_{pred} - d_{gt}, & -\delta < d_{pred} - d_{gt} < \delta \\ d_{gt} - d_{pred} - \delta, & d_{gt} - d_{pred} > \delta \end{cases}$$

$$L_{AD} = L_{clip} + \theta \sum_z d_{gt} + \beta \sum_z d_{pred} + \phi \sum_z \pi_{pred} + \theta \sum_z w_D \text{loss}_{Lipschitz}$$

$$L_D = L_{clip} + \theta \sum_z d_{gt} + \beta \sum_z d_{pred} + \phi \sum_z \pi_{pred} + \theta \sum_z w_D \text{loss}_{Lipschitz}$$

The overall loss function comprises multiple components, as defined in [S1](#) and [S2](#).

Let θ denote the AD model implicitly learning SD. Here z_i represents the latent vector embedding each shape while x_i and d_{gt} indicate the spatial coordinates and the corresponding ground truth distance. The β -AD was trained by computing the KL divergence D_{KL} between the learned latent distribution and the prior. To align the scale with L_{clip} and D_{KL} weights $w_{AD} = \frac{1}{\sqrt{2}}$ for the AD model and $w_D = \frac{1}{\sqrt{2}}$ for the D model were applied to the Lipschitz loss term.

An AD structure without an encoder was adopted; the rationale behind this design choice is detailed below.

reconstruction performance

reconstruction performance was compared for the AD and D models using chamfer distance, D-minimum matching distance, D and coverage. Other metrics as introduced by [Bang et al.](#) These metrics serve specific purposes. The formulas for CD, MMD and COV are as follows and respectively. Let $\mathcal{G}$ and $\mathcal{R}$ denote the sets of generated and reference point clouds respectively with $r \in \mathcal{R}$, $g \in \mathcal{G}$. The distance $D(\cdot, \cdot)$ between two point clouds is computed using either D or earth mover's distance. D measures similarity, D measures dissimilarity and COV measures diversity. COV serves as an indicator for mode collapse.

$$D(\mathcal{G}, \mathcal{R}) = \min_{g \in \mathcal{G}} \min_{r \in \mathcal{R}} \|g - r\| \quad \min_{r \in \mathcal{R}} \min_{g \in \mathcal{G}} \|r - g\|$$

$$D(\mathcal{G}, \mathcal{R}) = \frac{1}{|\mathcal{R}|} \min_{r \in \mathcal{R}} \sum_{g \in \mathcal{G}} D(g, r)$$

$$COV(\mathcal{G}, \mathcal{R}) = \frac{\arg\min_{r \in \mathcal{R}} \sum_{g \in \mathcal{G}} D(g, r)}{|\mathcal{R}|}$$

To evaluate both models experiments were performed on car shapes from ShapeNet and car wheels generated via deep generative models and parametric design. reconstructions were obtained using the trained models with sampled points used to compute metrics. As shown in Table [S1](#) the AD model consistently outperformed

the DD model for both car and wheel shapes with the DD mean indicating that the AD handles subtle variations effectively. Although the DD mean favored the AD the DD median was lower or the DD suggesting that mode collapse impacted the DD's performance particularly in smaller latent spaces (see also as shown in Fig. 4). Increasing the latent dimension in the AD led to difficulties in reconstructing thin structural res such as wheel rims while a smaller latent dimension allowed the model to capture fine features more comprehensively preserving a diverse and meaningful latent space.

Data	Structure	Latent dimension	Time	DD mean	DD median	DD	O
car	Auto decoder	10	h	0.85	0.85	0.85	0.85
		20		0.85	0.85	0.85	0.85
		30		0.85	0.85	0.85	0.85
	Auto decoder	30	d	0.85	0.85	0.85	0.85
heel	Auto decoder	10	h	0.85	0.85	0.85	0.85
		20		0.85	0.85	0.85	0.85
		30		0.85	0.85	0.85	0.85
	Auto decoder	30	d	0.85	0.85	0.85	0.85

Table 1: Training results

relatively short training time. The DD structure incorporates an encoder resulting in 10 to 100 times more parameters than the AD structure which contains 100 parameters. Both the AD and DD models were trained on 1000 paired data points for SD learning and the DD model additionally incorporated 1000 point-cloud samples into the training process. The slower training speed of the DD model is primarily due to its complex processing rather than just a larger parameter count comprising a β -Autoointnet and -net for global feature extraction. The DD

model performs additional operations like projecting point clouds onto two dimensions increasing processing time and its computational burden the model performs additional internal tasks such as projecting point clouds into two-dimensional planes. These operations consume considerable processing time, significantly challenging the overall training speed. Specifically, training the ED model on 30 samples required about 10 days on an Nvidia A100 GPU over 1000 epochs which is a significant drawback when rapid training is required. In contrast, the simplicity of the AD structure reduces computational overhead and training time dramatically it requires only about 10 hours over 100 epochs, highlighting its efficiency for rapid deployment.

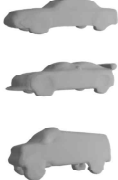
	Real	Auto decoder (dim: 5)	Auto decoder (dim: 128)	Encoder decoder
Car				
Wheel				

Figure 3: Reconstructed D-shapes for car and wheel datasets

periments

Dataset	Ob ecti e	periment	o data	Latent Dimension	se o e ral etwor
heel	max: stiffness	Data S nthesis			S nthesize the other t pes o data
	min mass	tremel Limited Data			plore shapes between data
ar	min D L	D Anal sis			Generate good- alit shapes or engineering anal sis
		tremel Limited Data			plore shapes between data

Table periment descriptions

n this section e periments were cond cted to demonstrate the no elt and ersatilit o the proposed methodolog artie larl this st d tilizes data-dri en methods to generate shapes with ario s eat res based on the training data lti-ob ecti e optimization was per ormed to le erage the abilit to e plore di erse shapes in the proposed approach The proposed methodolog s ersatilit was demonstrated thro gh e periments cond cted in the conte t o shape optimization across distinct data t pes D-based shape optimization and optimization between two shapes The e periment concerning the optimization between two shapes was cond cted sing car data and wheel data A brie description o the e periments is pro ided in Table periments cond cted in Section and were per ormed with a pop lation size o indi id als per generation iterating thro gh a total o generations Similarl the e perimental settings described in Section emplo ed a pop lation size o indi id als per generation o er generations

Shape Optimization across Distinct Data T pes

Traditional parametric shape optimization represents arbitrar shapes using a single set of parameters, potentially sacrificing some intrinsic degrees o reedom Similarl red cing the ll dimensionality o D inp t shapes to a compressed latent space ector ma res lt in some loss o in ormaton However, the learned latent space is designed to capture the most significant shape ariations which means it is more li el to preser e critical degrees

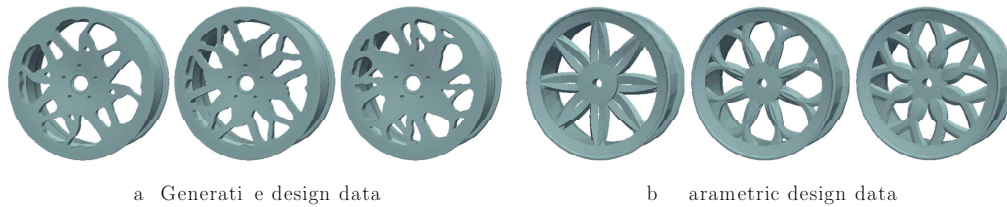


Figure 5: Different wheel design variations

of freedom across a broader range of shapes than conventional parametric representation techniques.

As seen in Figure 5, even when the same wheel is designed, data can be defined in a variety of ways. Defining various datasets as a single parametric set is impossible. As a result, no research on optimizing them has been conducted. The methodology of this study is based on data rather than parametric modeling, which is why it is not heavily dependent on the data generation process. To demonstrate this condition, experiments were conducted using a dataset comprising engineer-designed wheels and wheels generated by a deep generative model.

The selection process involved identifying wheel data with a spoke pattern composed of multiples of 5, allowing for a symmetrical shape achieved through a 72-degree rotation, considering the significant characteristic of cyclic symmetry in wheel data. In this study, stiffness is obtained by analyzing the natural frequencies of the wheels through modal analysis using the free-free method. The free-free method in modal analysis examines the natural frequencies and mode shapes of a structure in an unconstrained state, meaning the object has no fixed boundaries or supports. This is done by solving the eigenvalue problem derived from the system's equations of motion, which are based on its mass and stiffness properties. The natural frequencies correspond to the square roots of the eigenvalues, indicating the rates at which the structure vibrates naturally. This approach allows for an accurate assessment of the dynamic response of the structure without the influence of external constraints, which is crucial for predicting the behavior of components in real-world scenarios, especially in aerospace and mechanical applications.

Natural frequencies play a fundamental role in determining a structure's stiffness (with a direct relationship described by $f \propto \sqrt{k/m}$, where m represents the mass of the structure). This formula indicates that an increase in natural frequency corresponds to higher stiffness, whereas an increase in

mass yields lower stiffness. Natural frequencies indicate the rates at which the structure vibrates naturally when disturbed. Stiffness measures a structure’s resistance to deformation under an applied force, influencing how the structure responds to external loads and vibrations

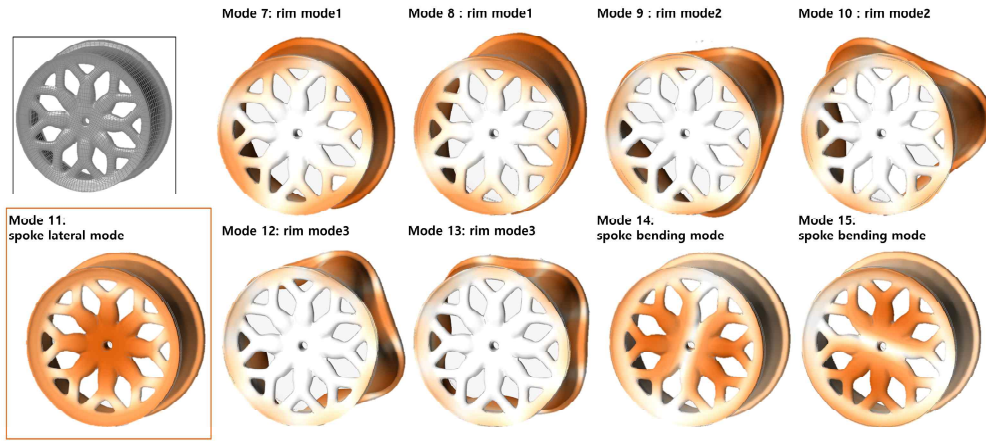


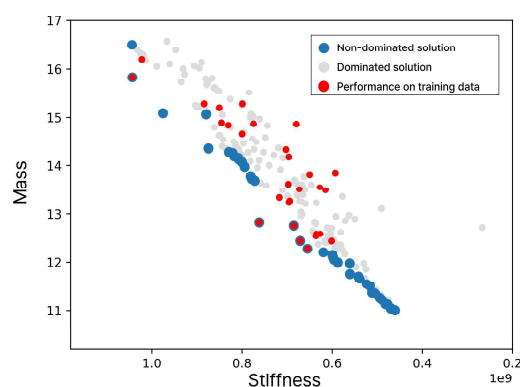
Figure 6: Modal analysis results: mode shapes across different modes

In this study, the stiffness was specifically calculated using the 11th mode, which is identified as the lateral mode of the spokes. The lateral mode involves vibrations that occur perpendicular to the wheel’s plane, directly affecting the structural integrity and performance of the wheel design.

$$m = \pi f$$

This experiment conducted multi-objective optimization with stiffness and mass as objectives. The results presented in Fig. 9 illustrate the evolution of shape designs positioned along the Pareto front across multiple generations. These outcomes demonstrate the proposed method’s ability to continuously explore data within a low-dimensional latent space rather than sampling and optimizing disconnected regions of the data space. The method successfully identifies meaningful candidate designs around the Pareto front, even when compared to the training data. Furthermore, Fig. 10 reveals that the proposed approach, being fundamentally data-driven, enables realistic

Exploration within a design space closely related to existing shapes to obtain the generated designs consistently exhibit high quality irrespective of their origin from either parametric or generative design methods. The experiment thus demonstrates the capability of the proposed methodology to effectively explore and optimize within a continuous low-dimensional data space rather than merely selecting solutions from isolated and discrete regions.



a Pareto front results using wheel samples



Stiffness max ← → min
 Mass max ← → min

b Non-dominated solutions from wheel samples

Figure Optimization experiment resulting two datasets

D-based Shape Optimization



Figure Diverse car shape expression

periments analyzing car aerodynamics were conducted as part of a generative model-based shape optimization study in this work the OpenFOAM solver was set up for an incompressible flow holds A eraged a ier-Stokes analysis sing air The simulation used SimpleFoam to capture the drag and lift forces generated as an external airflow, moving at 10 m/s, passes by the vehicle

3D car models were sourced from the ShapeNet dataset a widely used benchmark in 3D graphics from thousands of models those with clearly distinguished internal and external components and suitable mesh conditions for CFD analysis were selected The study included various car categories such as sedans sports cars cars with rear spoilers and sport utility vehicles

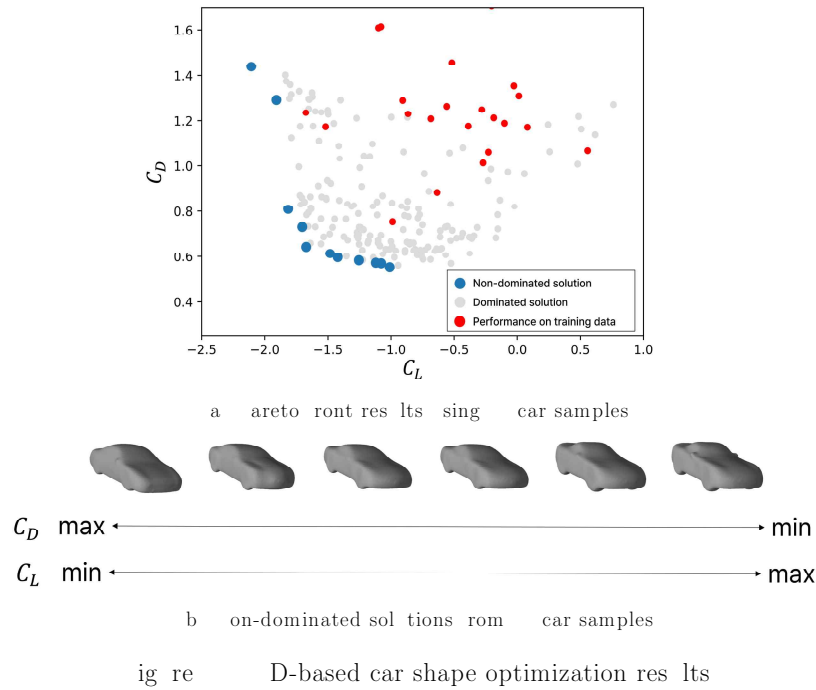
Unlike traditional approaches where explicit parameterization is required to represent and compare topological changes this data-driven methodology leverages generative models to directly capture the inherent shape features

This allows for the representation and comparison of topological variations solely based on the input data enabling the optimization process to preserve fine details that conventional parameterizations often miss

Using the OpenFOAM simulation framework a generative model was trained on a selection of ShapeNet car models Multi-objective optimization was performed to minimize the C_D and the C_L

The results are shown in Figure 4 As the generations progressed improved designs emerged and gradually converged toward the Pareto front following a trend similar to previous experiments Notably the generated candidates demonstrated superior aerodynamic performance compared to the training data Furthermore compared with the earlier wheel dataset study variations in car shapes exhibited a more pronounced influence on the objective

values resulting in a broader distribution along the Pareto front Figure 4b further highlights the diversity of optimized shapes spanning various vehicle categories from sports cars to sedans illustrating the model's capability to explore and generate diverse Pareto-optimal designs under the given objectives



Optimization between Two Shapes

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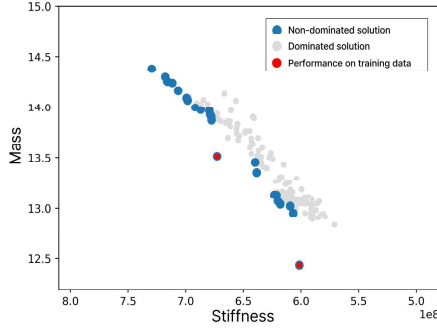
Table reconstr ction res lts or data

ilding on the o ndational wor described in Sections and this combined section e amines the application o the proposed optimization ramewor with a limited dataset sing onl two shapes or both wheels and cars n contrast to the pre io se periments which emplo ed a larger and more aried dataset o designs these e periments were designed to e al ate the methodolog s rob stness and adaptabilit nder e tremel lim- ited data ailabilit dential e perimental conditions to those described in Sections and were maintained to assess the optimization ramewor s

ability to derive meaningful design variations, with the only differences being a reduced number of data and a lower-dimensional latent space. The reconstruction accuracy obtained with this two-sample set up is summarized in Table

As shown in Figs. 4a and 4b the optimization algorithm established a coherent Pareto front even relying on just two data points. For the wheel shapes, the Pareto front based on stiffness and mass axes reveals that the model could generate diverse and engineering-relevant variations despite limited data. Noting that the model trained on only two wheel designs, exhibits a smooth interpolation along the Pareto front, effectively capturing design variations as if performing parametric adjustments in stiffness and mass. This behavior indicates that the A could simulate a continuum of structural adjustments between the limited initial designs, reflecting adaptability in exploring optimal shapes within minimal data constraints. Similarly, in the case of car shapes the optimization process generated significant aerodynamic variations between the two baseline designs. As shown in Fig. 4d the model maps meaningful shape changes that correlate with aerodynamic performance. The algorithm effectively balanced the aerodynamic objectives and physical design limits, achieving a range of optimized forms that reflect varying levels of aerodynamic efficiency within the specified constraints.

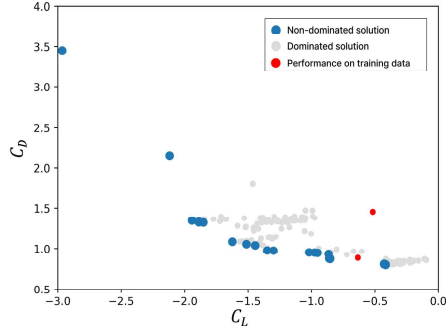
These findings underscore the strength of the proposed methodology in handling datasets with limited diversity while still producing reliable and relevant design options. Although the initial data diversity is constrained, the model effectively explored the potential design space, extracting patterns and structural characteristics that offer insight into performance optimization. This investigation thus affirms the adaptability of computational design methods under conditions of sparse data, showcasing that even with minimal input, significant design insights can be obtained.



a areto ront res lts sing two wheel samples



Stiffness max ← → min
Mass max ← → min



b areto ront res lts sing two car samples



C_D max ← → min
 C_L min ← → max

c on-dominated sol tions rom two wheel samples d on-dominated sol tions rom two car samples

ig re perimental res lts on e tremel limited data

oncl sion

This st d proposes an engineering per ormance-based D shape optimization process that o ercomes the drawbacks o e isting methodologies while incorporating the advantages o on entional DG -based shape optimization. tensi e h per-parameter t ning across ario s architect res was cond cted to select a s itable model or the proposed approach. le eraging a simple reg larization term and ad anced encoding techni es, a model was de eloped that is well-s ited or the limited dataset, a scenario typically considered one of the most challenging in the engineering field. Furthermore, three e periments were per ormed to highlight the advantages o this approach over conventional methods. The key findings of the study can be s mmarized as ollows:

Data S nthesis: Section details an e periment in which two distinct datasets are learned and optimized within the same latent space. This data-driven method, which does not require the explicit definition of parameters, enables exploration into previously undefined regions, where datasets ig a and b are s nthesized ill strated in ig b.



a Generated design with topology optimization



b Generated shapes using the proposed method

Figure 3: Comparison of shapes between the two methodologies

Generalizability: Multiple experiments were conducted using wheel data for structural analysis and car data for CFD, two of the most commonly employed numerical analyses in shape optimization. Section 4 demonstrates that the optimization process successfully explores non-dominated solutions that outperform the performance of the actual data.

Realizable Design: The proposed framework defines shapes by learning and extracting features from real data. As illustrated in Figure 3a, the data generated by topology optimization typically consist of a large amount of constructed data with pronounced straight branches. In contrast, Figure 3b shows shape expressions that closely resemble those observed in real-world applications.

The presented framework holds significant promise across two engineering applications. In domains such as car and wheel design, as employed in this study, the superiority of a shape cannot be defined solely in terms of engineering performance. These areas are inherently influenced by end-user preferences, with design iterations occurring through close collaboration between industrial designers and engineering designers who determine the overall form [71]. In this context, the proposed framework offers the advantage of exploring a data space that closely resembles real-world samples. This allows it to incorporate aesthetic considerations and manufacturability alongside quantitative engineering metrics. This capability paves the way for extending the framework to collaborative efforts within industrial design.

Moreover, the proposed approach can be integrated with recent advances in uncertainty quantification to develop task-aware surrogate models within an active learning paradigm. By defining objective values based on uncertainty rather than solely on engineering performance, the framework can facilitate more effective data sampling and contribute to the continuous improvement of surrogate model performance.

Despite these promising results, the proposed framework exhibits a notable limitation stemming from its strong dependence on training data. With ample data, the model can effectively generate a wide variety of design candidates. However, in scenarios where available training data are significantly limited, such as the extreme case discussed in Section 4.2, the performance range of the generated solutions becomes substantially constrained. Comparing performance distributions from Sections 4.1 and 4.2, it is evident that the distribution in Section 4.2 covers only a small design region. While increased data allows the exploration of broader design spaces, limited data imposes inherent interpolation constraints, highlighting the critical importance of selecting appropriate training samples.

Moreover, the metrics used to evaluate generative models have limitations. Most prior studies assume that a sufficient volume of training data is available when defining their problems. Consequently, metrics such as CD,

D and O are well-suited for evaluating large datasets but may not be appropriate in the “small data” regime defined here. Due to the use of a latent variable shape evaluation termed engineering performance, the broad spread of performance distributions permits the inference that the latent space is smoothly structured. However, D, D and O values alone do not guarantee that a generative model has learned a meaningful latent representation. Therefore, there is a need for metrics capable of evaluating whether a meaningful latent space can be defined even when only a small amount of data is available.

In this context, augmenting the limited dataset with strategically meaningful data points is essential to enhance both generative and predictive model performance. Defining what constitutes “meaningful data” for the model and empirically validating these definitions will be discussed as part of future research.

editorial contribution statement

Longmin won conceptualization Data curation formal analysis investigation methodology resources Software validation visualization and writing - original draft manuscript preparation project administration Supervision investigation funding acquisition writing - reviewing and editing

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