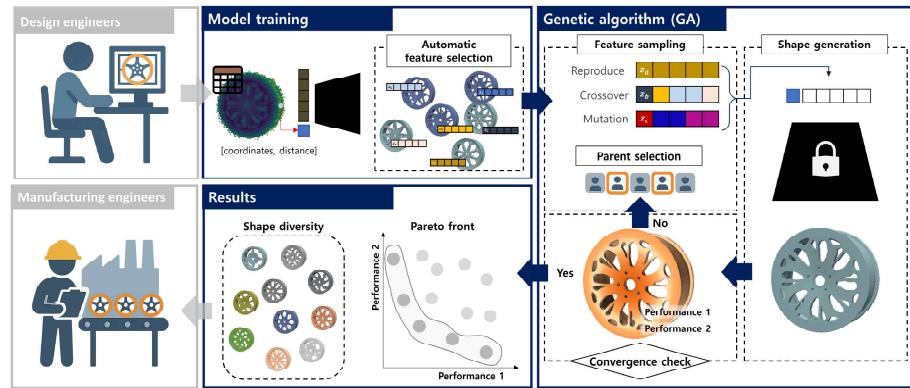


# Graphical Abstract

Three-dimensional Deep Shape Optimization with a Limited Dataset  
ongmin won amwoo ang



## Highlights

Three-dimensional Deep Shape Optimization with a Limited Dataset  
Jongmin Won, Junwoo Kang

Overcomes explicit parameterization limits using data-driven shape extraction

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

Generati e models ha e attracted considerable attention or their abilit to prod ce no el shapes Howe er their application in mechanical design re-mains constrained d e to the limited size and ariabilit o a ailable datasets This study proposes a deep learning-based optimization framework specif-call tailored or shape optimization with limited datasets le eraging positi-onal encoding and a Lipschitz reg larization term to rob stl learn geomet-ric characteristics and maintain a meaning l latent space Thro gh e tensi e e periments the proposed approach demonstrates rob stness generalizabil-ity and effectiveness in addressing typical limitations of conventional opti-mization frameworks. The validity of the methodology is confirmed through m lti-ob ecti e shape optimization e periments cond cted on di erse three-di-mensional datasets incl ding wheels and cars highlighting the model s ersatilit in prod cing practical and high- alit design o tcomes e en under data-constrained conditions

e words Signed Distance Function, Artificial Intelligence, Limited Dataset mplicit e ral epresentation Shape Optimization

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## ntrod ction

Artificial intelligence (AI) has shown significant achievements in various domains, including regression, classification and segmentation [1, 2]. Building pon these ad ancements research in mechanical design s ch as comp ter-

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

Deep generative models (DGs), such as the variational autoencoder (VAE) and 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, DGs guarantees data diversity by 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 features of 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 a 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 and compares that conventional parametric techniques and existing DG-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 2 introduces previous research

on shape optimization topolog optimization and shape optimization sing DG and disc sses data representation and deep learning architect re in the conte to D data Section pro ides an o er iew o the entire ramewor o this st d rom data collection to shape optimization Section e amines the originalit and alidit o the methodolog thro gh three shape optimization e periments inall Section presents concl sions and directions or t re wor

elated or s

### Shape Optimization ethod

#### arametric Shape Optimization

Data generated thro gh AD programs consists o combinations o aratio s geometric ariables which can be tilized as design parameters in the optimization process arametric 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 ob ecti e nction This method is widel sed in various engineering fields, including automotive, aerospace, electromagnetic and aco stic

arametric shape optimization has ad ained with s rrrogate modeling or 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 encaps lated b n merical characteristics perimen tal res lts indicate that the e tensi e design space and intricate parameter dependencies enable he ristic optimization methods s ch as the on-dominated Sorting Genetic Algorithm SGA- to o tper orm gradient-based approaches

or non-parametric data s ch as D meshes parameterization can be per ormed sing techni es li e pol c be mapping or ree- orm de ormati on These methods can be implemented relativ el easil and trans orm comple and detailed shapes rthermore when constr cting s rrrogate models mesh data can be represented as a graph and processed with graph ne ral networ s enabling the sol tion o more generalized problems Howe er a limitation o these methods is that depending on the resolution of the defined parameters, capturing fine details becomes challenging and the n mber o parameters increases

## Topolog Optimization-based Generati e 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 explores new shapes throughout the design process, from problem definition to detailed design. This approach streamlines the process by automatically 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 GA 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. Tensional 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 been developed according to the type of data intended. 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 architect res based on implicit ne ral representations as intro d ced b ar et al ha e been widel adopted These models are highl ersatile ser ing not onl as generati e models b t also as s r-rogate models. Their ability to perform auto-differentiation makes sensit it anal sis straight orward ma ing them well-s ited or capt ring local ariations This approach has been partic larl se 1 or ehicle aerod -namic optimization problems which t picall re ire high comp tational reso rces

O erall data-dri en deep generati e models disting ish themsel es rom topolog optimization-based generati e design in that the can e plore more realistic data distributions and discover unique configurations. However, they re ire large amo nts o data

	Topolog Optimization	arametric Shape Optimization	DG -based Shape Optimization	roposed method
arameterization	A tomatic	an al	A tomatic	A tomatic
nterpolation	n easible	n easible	ossible	ossible
on ergent possibilit	ad	Good	Good	Good
Training data	one	one	Large	Small minim m

Table comparison with other optimization methods

n s mmari Section is concisel represented b Table Altho gh DG -based shape optimization s ccess ll addresses the limitations o traditional topolog optimization and parametric shape optimization meth-ods, it still suffers from a critical drawback: requiring an extensive training dataset This st d addresses this iss e b proposing a rob st model that deli ers strong per ormance e en with limited datasets ma ing it partic -larl s itable or shape optimization applications Detailed descriptions and e planations are pro ided in Section

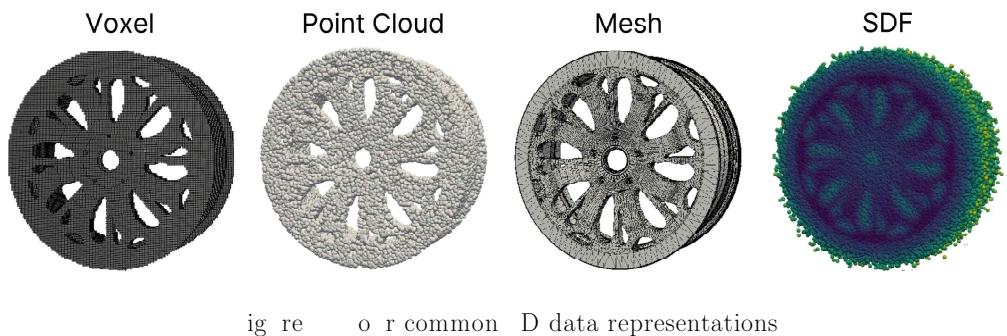


Figure 1 shows four common 3D data representations:

### Deep Learning or 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 voxel, point cloud, and mesh representation as shown in Figure 1.

Voxel 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 voxel approach to represent 3D shapes can lead to memory issues. Furthermore, representing a 3D shape as a voxel 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 blunt.

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 or learning D 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 SD being a prominent example. This can be expressed in terms of the coordinates in space as the signed distance  $s$  to the surface as shown in. The SD represents the shortest distance from a point to the shape 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.

$$SD \quad s \quad S$$

The surface of a shape represented by SD can be expressed as the isosurface of  $SD = 0$  and this can be converted into a discretized surface using algorithms such as marching cubes.

### Implicit visual representation

Implicit representations such as SD enable implicit learning where coordinates serve as inputs to an A 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 D 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 SDs and learning them implicitly several models have been introduced for shape manipulation. These include D alSD which adds a coarse network for shape manipulation and A-SD which disentangles the latent space of articulated objects. All of these models share a common encoder AD structure without a separate encoder. Unlike many generative models that reduce data dimension within a bottleneck structure, these models do not have a separate encoder or data compression instead the AD inputs both coordinates and latent code into the model and back propagation optimizes latent code within the model.

Encoder-decoder D models that utilize encoders such as point net to compress data exist. These structures create latent codes through an encoder which has been used to handle implicit data. The work by Eng 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 volumes transforming nested 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 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 SDF network to predict the distance.

## Methodology

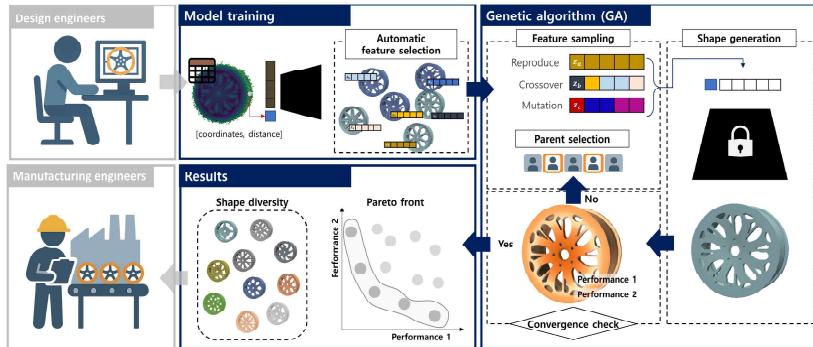


Figure 1: Overview of the proposed optimization framework.

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 10-wheel and 10-car data from both topology optimization and parametric design methods was carefully selected to demonstrate that optimization can be effective even with limited data. Preprocessing then ensured data valid through checks for mesh flips and watertightness [60], followed by centering, normalization and sampling surface-adjacent points with corresponding SDF 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	sed
parent selection	Toournament selection
rosso er	Simulated binary crossover
tation	polynomial mutation

Table 2: Used operators

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 refine the results, converging to suboptimal solutions. This approach is well-suited for complex optimization challenges, enabling a-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 discover diverse shape designs.

#### Shape Generation Simulation

Using latent codes produced by the optimization algorithm, the decoder generated new shapes by producing a Surface Definition (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 Open OA. 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 hec

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

### Network Architect re

Mechanical design products have boundary conditions such as load and fixed conditions, resulting in minimal differences among the data. Therefore, it is important to generate models over 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 fine 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 MLP model must accurately learn the features of the dataset even with sparse data while employing a meaningful latent space. Positional encoding and Lipschitz regularization terms have been introduced to address these issues.

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

$$\gamma p \quad \sin(\pi p) \quad \cos(\pi p) \quad \sin(\pi p)^L \quad \cos(\pi p)^L$$

$p$  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 enables the model 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 encodings 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  $L_i$  as represented by the layer equation:

$$eL_i = b_i / \text{normalization}_i = \ln(e^i)$$

For all layers of the decoder, the Lipschitz layer normalizes the weight matrix  $b_i$  of each  $i$ -th linear layer using trainable Lipschitz bounds  $\ln(e^i)$  as shown in:

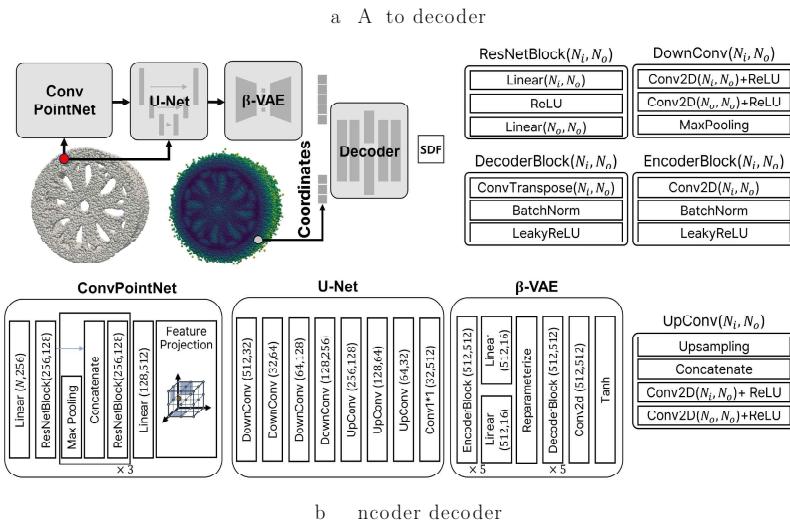
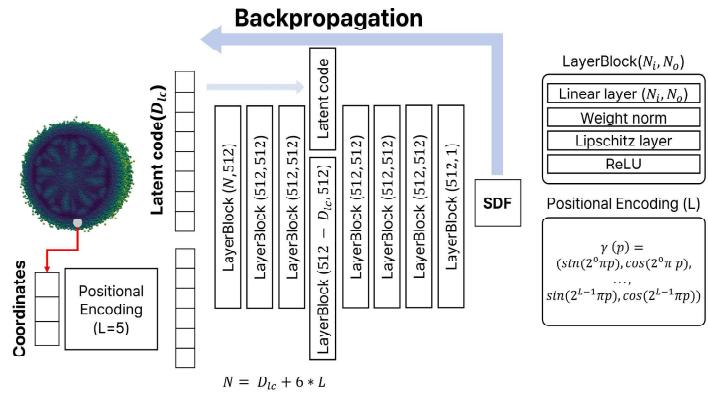
$$\text{loss}_{\text{Lipschitz}} = \frac{1}{i} \sum_{i=1}^I \ln(e^i)$$

The overall Lipschitz bound for the network is determined by the product of the individual Lipschitz constants  $\ln(e^i)$  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 without an encoder and an ID structure that integrates a point-set-based encoder  $\phi$ , as shown in Figure 3. This encoder inputs point cloud data  $\pi_{\text{ped}}$  and extracts latent features. Both models are trained using a latent space regularization term and a truncated L1 loss to measure discrepancies between predicted and true SDF values. The truncated L1 loss, a modification of standard L1 loss, truncates both positive and negative outliers to limit extreme deviations while preserving sensitivity within a specified range ( $\delta$ ). As illustrated in the experiments,  $\delta$  was set to 0.05 and  $\beta$  was set to 0.01.



b encoder decoder

fig re model architect res

$$L_{clip} = \frac{\max(d_{pred} - \delta, \delta)}{d_{pred} - d_{gt}} \cdot \frac{d_{gt} - \delta}{\delta - \min(d_{pred}, \delta)}, \quad -\delta < d_{gt} < \delta, \quad d_{gt} > \delta.$$

$$L_{AD} = L_{clip}(\theta, z, d_{gt}) - \beta \|D_L(\phi(z, \pi_{ped})) - z\|_2 \text{w}_{AD} \text{loss}_{\text{Lipschitz}}$$

$$L_D = L_{clip}(\theta, z, d_{gt}) - \beta \|D_L(\phi(z, \pi_{ped})) - z\|_2 \text{w}_D \text{loss}_{\text{Lipschitz}}$$

The overall loss function comprises multiple components, as defined in  $\mathbf{s}$  and

Let  $\theta$  denote the A model implicitl learning SD. Here  $z_i$  represents the latent vector embedding each shape while  $d$  and  $d_{gt}$  indicate the spatial coordinates and the corresponding gro nd tr th distance. The  $\beta$ - A was trained b comp ting the  $L$  di ergence  $D_L$  between the learned latent distrib tution and the prior. To align the scale with  $L_{clip}$  and  $D_L$  weights o wAD  $\times \gamma$  or the AD model and  $w_D \times \gamma$  or the D model were applied to the Lipschitz loss term.

An AD str ct re witho t an encoder was adopted the rationale behind this design choice is detailed below

#### econstr ction per ormance

econstr ction per ormance was compared or the AD and D models sing cham er distance  $D$  minim m matching distance  $D$  and co erage  $O$  metrics as introd ced b ang et al. These metrics serve specific purposes. The formulas for CD, MMD and COV are as s and respecti el. Let  $g$  and  $r$  denote the sets o generated and re erence point clo ds respecti el with  $r_g$ . The distance  $D_{\cdot \cdot}$  between two point clo ds is comp ted sing either D or earth mo er s distance.  $D$  meas res similarit  $D$  meas res alit and  $O$  meas res di ersit.  $O$  ser es as an indicator or mode collapse

$$D_{g,r} = \min_{\substack{r \\ g}} \min_{\substack{g \\ r}} |g - r|$$

$$D_{g,r} = \frac{\min_{\substack{r \\ g}} D(g, r)}{\min_{\substack{r \\ g}} D(g, r)}$$

$$O_{g,r} = \frac{\operatorname{argmin}_{\substack{r \\ g}} D(g, r)}{g}$$

To e al ate both models e periments were per ormed on car shapes rom Shape et and car wheels generated ia deep generati e models and parametric design econstr ctions were obtained sing the trained models with sampled points sed to comp te met- rics. As shown in Table the AD model consistentl o tper ormed

the D model or both car and wheel shapes with the D mean indicating that the AD handles subtle variations effectively. Although the D mean favored the AD the D median was lower or the D suggesting that mode collapse impacted the Ds performance particularly in smaller latent spaces whereas shown in figure increasing the latent dimension in the AD led to difficulties in reconstructing thin structures 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	D mean	D median	D	O
car	A to decoder	_____	h	_____	_____	_____	_____
	encoder decoder	_____	d	_____	_____	_____	_____
heel	A to decoder	_____	h	_____	_____	_____	_____
	encoder decoder	_____	d	_____	_____	_____	_____

Table Training results

elatively short training time.

The D structure incorporates an encoder resulting in times more parameters than the AD structure which contains parameters. Both the AD and D models were trained on paired data points or SD learning and the D model additionally incorporated point-coded samples into the training process.

The slower training speed of the D model is primarily due to its complex processing rather than having a larger parameter count comprising a  $\beta$ -A point set and a set of global feature extraction for the D

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 10 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 10 epochs, highlighting its efficiency for rapid deployment.

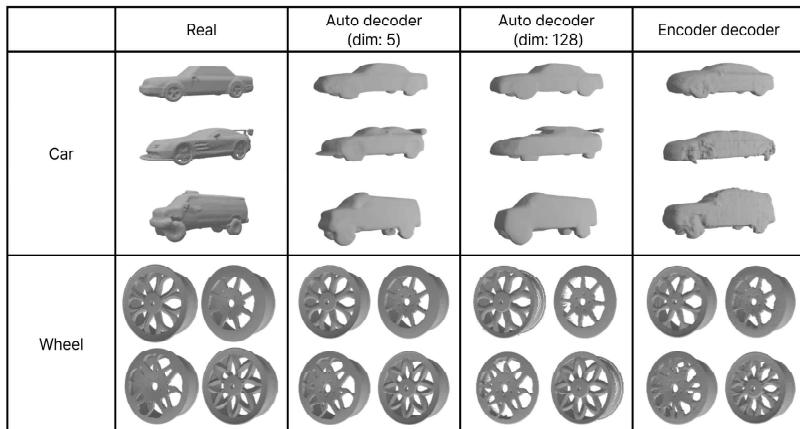


Figure 4: Reconstructed 3D shapes for car and wheel datasets

## periments

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

Table experiment descriptions

In this section experiments were conducted to demonstrate the novelty and versatility of the proposed methodology. Specifically, this study utilizes data-driven methods to generate shapes with various features based on the training data. Multi-objective optimization was performed to leverage the ability to explore diverse shapes in the proposed approach. The proposed methodology's versatility was demonstrated through experiments conducted in the context of shape optimization across distinct data types. D-based shape optimization and optimization between two shapes. The experiment concerning the optimization between two shapes was conducted using car data and wheel data. A brief description of the experiments is provided in Table . The experiments conducted in Section and were performed with a population size of individuals per generation, iterating through a total of generations. Similarly, the experimental settings described in Section employed a population size of individuals per generation over generations.

### Shape Optimization across Distinct Data Types

Traditional parametric shape optimization represents arbitrary shapes using a single set of parameters, potentially sacrificing some intrinsic degrees of freedom. Similarly, reducing the dimensionality of input shapes to a compressed latent space vector may result in some loss of information. However, the learned latent space is designed to capture the most significant shape variations, which means it is more likely to preserve critical degrees

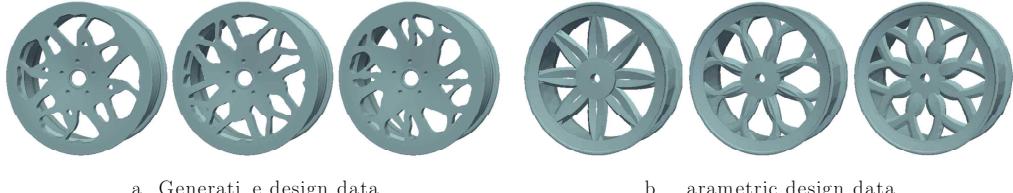


Figure 5: Different wheel design variations

o 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 allowing for asymmetrical shape achieved through a 180-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 assumes 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  $\omega_n = \sqrt{\frac{k}{m}}$  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.

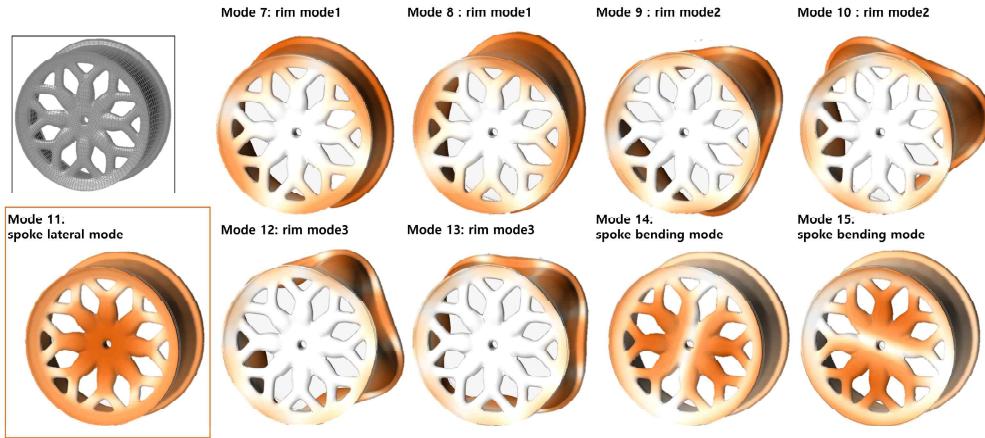


Figure 6: Modal analysis results: mode shapes across different modes

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 Figure 6 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, it reveals that the proposed approach being fundamentally data-driven enables realistic

Exploration within a design space closest related to existing shapes obtainable the generated designs consistently exhibit high stiffness 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.

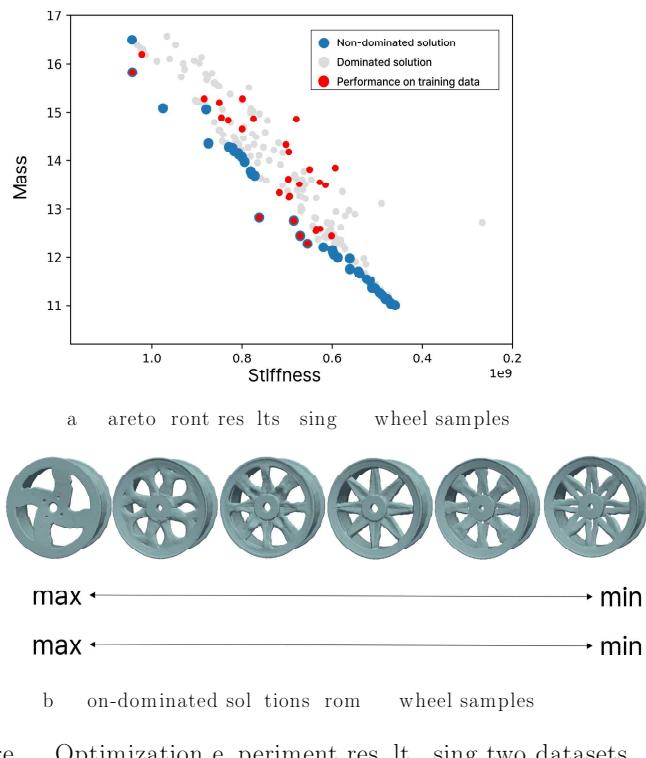


Figure 4 Optimization experiment results using two datasets

### D-based Shape Optimization



Figure 5 Diverse car shape expression

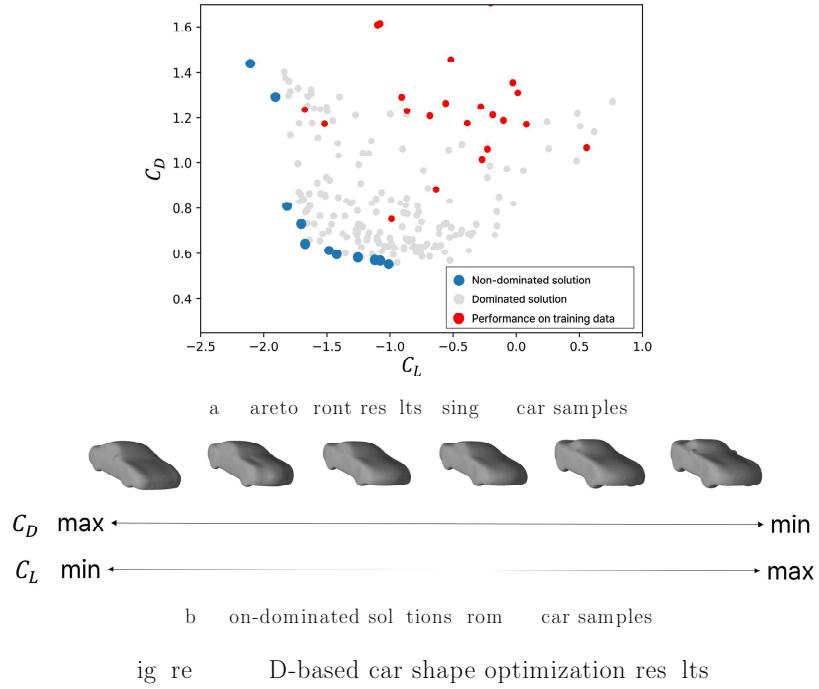
periments analyzing car aerodynamics were conducted as part of a generative model-based shape optimization study. In this work, the Open OA solver was set up for an incompressible flow. A grid of aier-Stokes analysis using air. The simulation used SimpleFoam to capture the drag and lift forces generated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

3D car models were selected from the ShapeNet dataset, a widely used benchmark in 3D graphics. From the thousands of models, those with clearly distinguished internal and external components and suitable mesh conditions for 3D 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 Open OA simulation framework, a generative model was trained on a selection of ShapeNet car models. Multi-objective optimization was performed to minimize the  $D$  and the  $L$ .

The results are shown in Figure 1. 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, the variations in car shapes exhibited a more pronounced influence on the objective values resulting in a broader distribution along the Pareto front. Figure 2 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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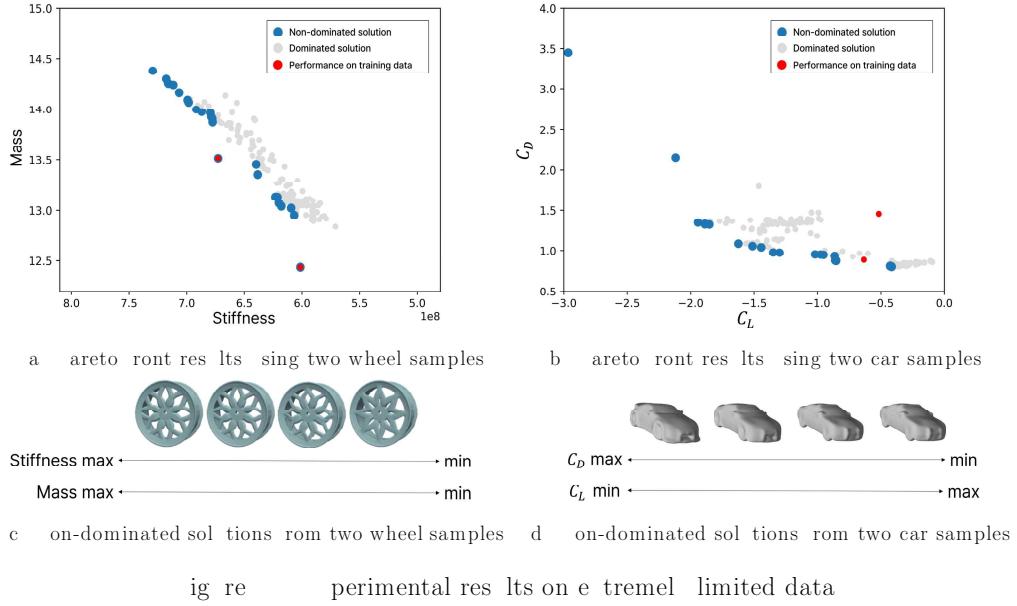
Table 1: Comparison of results obtained from the proposed framework.

Building on the foundational work described in Sections 3 and 4, this combined section examines the application of the proposed optimization framework with a limited dataset, using only two shapes or both wheels and cars. In contrast to the previous experiments which employed a larger and more varied dataset of designs, these experiments were designed to evaluate the methodology's robustness and adaptability under extremely limited data availability. Identical experimental conditions to those described in Sections 3 and 4 were maintained to assess the optimization framework'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 is summarized in Table

As shown in Figs. 5a and 5b, the optimization algorithm established a coherent Pareto front even relying on just two data points or training on 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. In Fig. 5c, 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 model 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. 5d, 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.

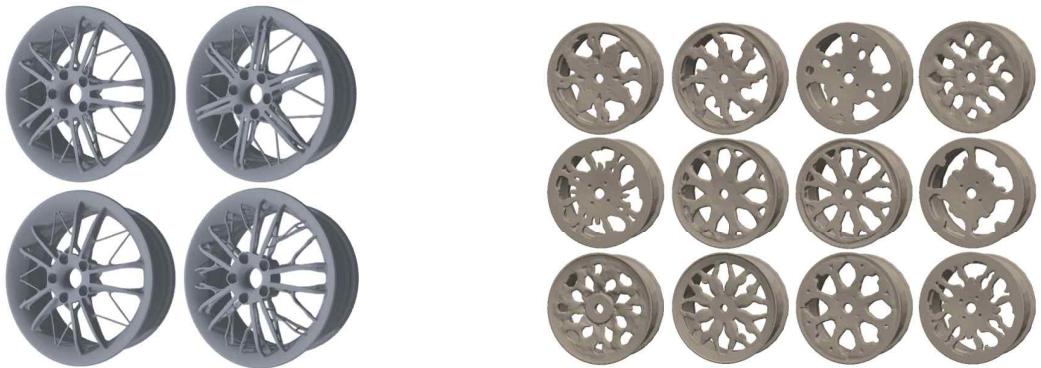
These findings underscore the strength of the proposed methodology in handling datasets with limited diversity while still producing reliable and relevant design outputs. Although the initial data diversity is constrained, the model effectively explored the potential design space, extracting patterns 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.



## Conclusion

This study proposes an engineering performance-based D shape optimization process that overcomes the drawbacks of existing methodologies while incorporating the advantages of conventional DG-based shape optimization. Tensile hyper-parameter tuning across various architectures was conducted to select a suitable model for the proposed approach. Incorporating a simple regularization term and advanced encoding techniques, a model was developed that is well-suited for the limited dataset, a scenario typically considered one of the most challenging in the engineering field. Furthermore, three experiments were performed to highlight the advantages of this approach over conventional methods. The key findings of the study can be summarized as follows:

Data Synthesis Section details an experiment 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 (a) and (b) are synthesized and illustrated in Fig. b.



a Generated design with topological optimization      b Generated shapes using the proposed method  
Figure 4 Comparison of shapes between the two methodologies

Generalizability: ample experiments were conducted using wheel data or structural analysis and car data or D two of the most common employed numerical analysis in shape optimization. Section demonstrates that the optimization process successfully explores non-dominated solutions that optimize 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 4(a), the data generated by topological optimization typically consists of a large amount of structured data with pronounced straight branches. In contrast, Figure 4(b) shows shape generations 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.

oreover 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 3, the performance range of the generated solutions becomes substantially constrained. Comparing performance distributions from Sections 3 and 4 it is evident that the distribution in Section 4 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 quantitative shape evaluation termed engineering performance the broad spread of performance distributions permits the inference that the latent space is smooth and structured. However D, D and O 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 the research.

## edit a thorship contrib tution statement

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