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Dynamic inverse design of broadband metasurfaces with synthetical neural networks

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Abstract: For over 35 years of research, the debate about the systematic compositionality of neural networks remains unchanged, arguing that existing artificial neural networks are inadequate cognitive models. Recent advancements in deep learning have significantly shaped the landscape of popular domains, however, the systematic combination of previously trained neural networks remains an open challenge. This study presents how to dynamically synthesize a neural network for the design of broadband electromagnetic metasurfaces. The underlying mechanism relies on an assembly network to adaptively integrate pre-trained inherited networks in a transparent manner that corresponds to the metasurface assembly in physical space. This framework is poised to curtail data requirements and augment network flexibility, promising heightened practical utility in complex composition-based tasks. Importantly, we accurately capture the intricate coupling effects between different metasurface segments. We exemplify our approach for two broadband metasurface inverse design problems, reaching accuracies of 96.7% and 95.5%. Along the way, we highlight the importance of suitably formatting the spectral data to capture sharp spectral features. This study marks a significant leap forward in inheriting pre-existing knowledge in neural-network-based inverse design, improving its adaptability for applications involving dynamically evolving tasks.

28 Introduction

29 The endeavor to utilize available labels or observations for formulating decisions in the face of unseen
30 incentives represents a common goal within the realm of deep learning¹. Its success, comparable to
31 a model of the mind, has not materialized overnight. The landscape of artificial intelligence and deep
32 learning has, until now, undergone significant evolution. Recent strides, especially in the domain of
33 deep neural networks, have showcased remarkable progress in replicating human-like reasoning and
34 cognition. Fueled by extensive datasets and advanced architectures, deep learning models have
35 attained exceptional performance across natural language processing², image recognition³, and
36 reinforcement learning⁴. These contemporary models demonstrate the capacity to grasp intricate
37 patterns, recognize hierarchies, and exhibit reasoning capabilities once considered beyond the reach
38 of artificial systems. This transformative journey parallels the integration of machine learning into
39 various fields, notably photonics, where metasurfaces emerge as a prominent representative⁵⁻¹⁸.
40 Metasurfaces, imbued with the power of machine learning, have proven instrumental in optimizing
41 device performance. This has led to the development of highly efficient metasurfaces and plasmonic
42 structures, enabling precise control of light in ways once deemed exceptionally challenging¹⁹⁻²⁸. In the
43 realm of metasurfaces, deep learning assumes a pivotal and indispensable role, serving as the linchpin
44 in the process of uncovering intricate patterns and recognizing hierarchies. This symbiotic relationship
45 empowers metasurfaces with the finesse needed to intricately control the behavior of light. This not
46 only marks a paradigm shift in photonics but also opens up diverse avenues for applications across
47 telecommunications, imaging, sensing, and beyond²⁹⁻⁴¹.

48 However, amidst these remarkable achievements, it is crucial to acknowledge that a fundamental
49 challenge raised by Fodor and Pylyshyn in 1988 persists – they asserted that artificial neural networks
50 lack the systematic compositionality necessary to be viable models of the human mind⁴². This
51 inherent lack of compositionality further manifests in deep learning models tailored for metasurface
52 design, often resulting in task-specific approaches. Each unique design challenge necessitates a
53 distinct architectural approach, leading researchers to embark on fresh journeys, developing novel
54 networks, and adapting the learning process. This iterative process can be time-consuming and
55 resource-intensive, impeding the swift exploration and optimization of metasurface designs for
56 diverse applications. Furthermore, deep learning models are notorious for their "black-box" nature,

57 making it arduous to decipher their decision-making processes and comprehend the underlying
58 physical mechanisms. This lack of interpretability introduces uncertainty in critical applications,
59 restricting the capacity to derive valuable insights into the fundamental principles governing
60 metasurface behavior. In addition, another requisite for effective deep learning is the availability of
61 extensive datasets. Acquiring such vast, well-labeled datasets specific to metasurface behaviors can
62 be a formidable undertaking, particularly in specialized or niche applications. Often, we must resort
63 to generating synthetic data or resorting to limited datasets, which may not fully capture the
64 intricacies of real-world scenarios. Given the limitations, a multi-capacity deep learning framework is
65 highly desirable, robustly handling diverse metasurface design tasks by adapting knowledge from
66 related examples to overcome data scarcity, efficiently exploring various functionalities, and
67 enhancing interpretability through model visualization.

68 To address the lack of systematic compositionality, we explore a modular approach to metasurface
69 inverse design with neural networks that inherits knowledge from neural networks previously trained
70 for the inverse design of different segments of which the new target metasurface is composed. The
71 resulting synthetical neural network inherits and amalgamates valuable knowledge from prior designs,
72 akin to passing down essential knowledge from the parent generation to the next generation. This
73 eco-conscious method capitalizes on pre-existing knowledge to streamline the design process and
74 significantly alleviate the cost of training the neural network. The synthetical neural network can also
75 be termed a knowledge-inherited network⁴³ or a genetic neural network.

76 The difficulty of inverse-designing metasurfaces with a modular approach that inherits inverse-design
77 networks for different segments of the metasurface lies in capturing the intricate mutual-coupling
78 effects between different segments. Given the resonant nature of the metasurface segments, the
79 combination of reflection spectra of individual segments into that of a composite metasurface is
80 highly non-trivial. Especially sharp spectral features cannot be predicted intuitively. Previous
81 preliminary work on knowledge-inherited NNs recently presented in Ref.⁴³ was limited to the
82 monochromatic regime and deliberately limited coupling effects as much as possible in order to then
83 neglect them in the forward model. In contrast, here we tackle the challenging problem of capturing
84 the broadband coupling effects between and within different metasurface segments. Moreover,
85 Ref.⁴³ only explored the regular tiling of metasurface segments in an array-like fashion whereas we

86 consider more intricate segmentations of the final metasurface in the present paper where one
87 segment is physically surrounded by another, which can be expected to yield more complex coupling
88 effects.

89 To illustrate broadband inverse design with a synthetic neural network despite challenging coupling
90 effects between different metasurface segments, we here design three "parent" components (one
91 square and one annular) and three corresponding "parent" neural networks that achieve an
92 impressive average accuracy of 99.6%. These "parent" components and "parent" networks are
93 compiled into a gene library. For a new "offspring" metasurface, we nest the parent components in
94 physical space, and then assemble the corresponding "parent" neural networks into an "offspring"
95 network. Here, we present examples of assembling two and three components from the gene library,
96 where the accuracy of the "offspring" neural network is recorded at 96.7% and 95.5%, respectively,
97 forming a sharp contrast with the accuracy of the conventional network at 38.5%. We expect our work
98 to play a significant role in photonics design by improving its adaptability as well as its frugality with
99 respect to scarce resources (compute power, time and energy consumption).

100 **Results**

101 **Notion of synthetic neural network.** In the domain of metasurfaces design and intelligent
102 application, a central focus resides in the meticulous structural design of meta-atoms, known as
103 inverse design. This approach is dedicated to crafting structures that meet stringent requirements or
104 predefined performance criteria in terms how they manipulate electromagnetic waves. The
105 methodology involves the intricate adjustment of geometric shapes, material properties, or
106 metasurface distributions to achieve targeted reflective, transmissive, or absorptive characteristics
107 within designated frequency ranges. In recent years, deep learning has emerged as a prominent
108 optimization method for this kind of inverse-design task. Artificial neural networks, inspired by the
109 biological nervous system, consist of interconnected artificial neurons. Each neuron processes input
110 through weighted mechanisms, contributing to the generated output (Fig. 1). Leveraging the robust
111 interconnectivity between nodes, neural networks facilitate automated processing and predictions
112 for complex tasks. However, in conventional deep learning-based metasurface inverse design, the
113 neural network is typically structured for a specific task. When transitioning to a new task, the pre-
114 trained neural network, labeled data, and all training outcomes must be discarded. Notably, the

115 disposal of labeled data emphasizes the necessity to reset the learning process entirely, posing a
116 time-consuming challenge, especially for metasurfaces relying on simulation-generated data. Here,
117 we seek to overcome this limitation with a synthetic neural network. This method decomposes the
118 solution space, assigning each split subproblem to its corresponding neural network. Ultimately, an
119 overarching network assembles all sub-networks. When confronted with an entirely new task, the
120 selection of suitable neural networks (NNs) and their assembly in a specific order enables the rapid
121 synthesis of an entirely new synthetic neural network. This is exemplified by the free assembly of
122 NN 1/2/4 and the addition of a new NN 5 in Fig. 1. Further, due to the drastic reduction in the solution
123 space, the data required for sub-networks significantly decreases, and the complexity of their
124 network architecture also decreases. This not only greatly alleviates the difficulty of exploring the
125 original solution space, but also endows the neural network-based inverse-design process with a
126 recycling feature, attributed to the flexible assembly characteristics among its sub-networks.

127 Our modular approach to composing a NN for metasurface inverse design resembles the concept of
128 transfer learning insofar as it reuses NNs previously trained for related but different tasks. Transfer
129 learning maintains the architecture of a previously trained NN and retrains its weights for the new
130 task. Therefore, it does not offer flexibility to combine knowledge learned by multiple NNs previously
131 trained on related sub-tasks. In contrast, our modular approach allows our synthesized NN to inherit
132 and combine knowledge from multiple NNs previously trained on related tasks that we consider
133 relevant based on our understanding of the physical problem. Therefore, we keep the architecture
134 and weights of the NNs previously trained on various related sub-tasks fixed (we refer to them as
135 INNs). We integrated these INNs into a synthetic NN composed of an ASNN followed by the INNs. By
136 training the ASNN we only learn how to combine the inherited knowledge from various INNs. This
137 methodology makes the NN synthesis transparent and has a clear relation to the metasurface
138 assembly in the physical reality. By efficiently combining inherited knowledge, our approach strongly
139 reduces the amount of required training data as well as the computational effort required for training.

140 **Architecture of synthetic neural network.** For concreteness, we consider the design of a reflective
141 1-bit coding metasurface that consists of a metallic pattern on top of a dielectric substrate with a
142 thickness of 2 mm and a relative permittivity of $3.5+0.00245i$, backed by a metallic ground plane. The
143 metallic pattern can be understood as a matrix of elements of size $10 \times 10 \text{ mm}^2$ that are either

144 metallized or not. The goal of the inverse design is to decide which elements should be metallized for
145 a desired electromagnetic response. As metasurface inverse design is demand-driven, in traditional
146 machine learning-based optimization, the input typically comprises the reflection spectrum (S_{11}
147 parameter), while the output corresponds to the metallic resonant surface (Fig. 2a). When
148 encountering a new task (Target 2), a completely new traditional neural network (TNN 2) is often
149 required. Here, the resonant surface can be discretized into pixel blocks represented as matrix \mathbf{R}_M ,
150 where M represents the number of pixel blocks ($M = 10$ in our case), and each block exhibits a
151 physical size of p/M , where the blue/ yellow color indicates the absence/presence of metal in that
152 block.

153 Our optimization strategy takes an unconventional route. Initially, the targeted "offspring"
154 metasurface is partitioned into two "parent" components, a square \mathbf{R}_8 and one annular ring \mathbf{R}_M^N
155 with the ring width of 2 mm, where M/N denote the outer/inner contour side length, respectively.
156 Subsequently, we construct and train inverse design networks for each "parent" component,
157 cataloging them in a "gene" library, each of which can be referred to as an inheritance neural network
158 (INN). The amalgamation of all INNs is then coordinated and deployed by an assembly neural network
159 (ASNN), with the S_{11} parameter of "offspring"/"parent" component representing its inputs/outputs.
160 The overall network composed of the ASNN and the INNs for a specific inverse-design task is referred
161 to as the synthetic neural network. When confronted with a novel task, such as \mathbf{R}_{10} in our case,
162 the adaptation process involves the addition of a new INN 2 and a corresponding ASNN (Fig. 2b). This
163 addition facilitates the assembly of two parent neural networks to effectively address the new task,
164 obviating the need for an extensive overhaul of the entire network architecture or the collection of
165 a large volume of \mathbf{R}_{10} -specific data. It is noteworthy that despite the introduction of new networks
166 (INN 2 and ASNN), each additional INN can be judiciously repurposed, and the structural adjustments
167 required for the ASNN are minimal. This efficiency underscores a reduced investment of time and
168 resources in network design. Furthermore, due to the decomposition of metasurface inverse design
169 into smaller subproblems, the data requirements are substantially diminished, simplifying the
170 problem-solving process for the corresponding inverse-design tasks.

171 An INN is employed to approximate the relationship between the S_{11} parameters of a given
172 "parent" component and its respective metallic patterns \mathbf{R} . The S_{11} parameters are significantly

173 influenced by the metallic structure, often leading to multiple sharp resonant features. To ensure
174 that our INN can properly process the S_{11} spectra, we extract the contour profiles of the S_{11}
175 parameters and resize them into 100 x 100 images, as detailed in the subsequent section. In this
176 configuration, the INN takes a 100 x 100 x 2 S_{11} image as input, where the two channels in the third
177 input dimension represent the real and imaginary components. The output is binarized to yield the
178 corresponding resonant metallic surface in line with the physical 1-bit coding constraint. INN 1/2
179 generate \mathbf{R}_8 and \mathbf{R}_{10}^8 , respectively. To tackle the non-uniqueness challenge of inverse-design
180 (multiple resonant surfaces can yield nearly identical S_{11} parameters), the so-far described INN
181 architecture acts as an encoder that is complemented by a decoder. The decoder is a forward design
182 network (FDN) which maps the metasurface \mathbf{R} to S_{11} images. Both encoder and decoder are
183 structured as convolutional neural networks (CNNs) and arrange in an encoder-decoder configuration
184 (Fig. 2c). Overall, the encoder-decoder network seeks to approximate the identity function. The loss
185 function quantifies the discrepancy between the input and output S_{11} images. We evaluate the loss
186 function using the mean square error (MSE) metric, in line with established practices in deep learning,
187 and we train the encoder-decoder network using a standard gradient descent algorithm⁴⁴.

188 Operating as an essential component within the structural assembly phase, the ASNN assumes a
189 critical role in discerning the coupling laws governing interactions among structural constituents. The
190 ASNN's input is a 100 x 100 x 2 S_{11} image. The ASNN's output with dimensions of 100 x 100 x 4
191 corresponds to two S_{11} images, one for each of the two "parent" components. These two S_{11}
192 images represent the reflection spectra that the two components of which the final metasurface will
193 be composed should yield. Therefore, the ASNN must "understand" the intricate coupling effects
194 between these two components. The two S_{11} images output by the ASNN hence serve as inputs for
195 the INNs. Regarding the ASNN architecture, we heuristically found that it is helpful to structure the
196 ASNN with an encoder and decoder part comprising seven convolutional layers (encoder part) and 6
197 deconvolutional layers (decoder part). However, unlike the INNs, the ASNN does *not* seek to
198 approximate an identity function. The ASNN is trained with triplet data where each example includes
199 the reflection spectrum of a given metasurface and the reflection spectra of its two constituent
200 components. The loss function is again defined as an MSE that quantifies the discrepancies between
201 the ground truth and the predicted outcomes for the reflection spectra of the two metasurface

202 components (see Materials and Methods).

203 **Pre-processing of spectral data.** Due to the inherent physical characteristics of resonant structures,
204 rapid spectral variations typically emerge near resonances, resulting in sharp resonant features that
205 are highly sensitive to minor structural alterations (Fig. 3a). We observed that simply discretizing the
206 spectral data and stacking its real and imaginary components before inputting it into the ASNN is not
207 a suitable data format because it does not yield a satisfactory ASNN performance. This observation
208 makes sense because the ASNN is based on a CNN architecture which is specialized in processing 2D
209 image inputs. Specifically, in Fig. 3b we illustrate the results of training the ASNN with 5,000 samples
210 of the S_{11} parameter which are formatted as 2002 x 2 arrays, where the first dimensions represent
211 frequency and the second dimension corresponds to real and imaginary parts. Examination of
212 randomly selected test samples highlights a notable discrepancy between predicted (dotted line) and
213 actual values (solid line), particularly near resonances. Evaluation using the Pearson correlation
214 coefficient (PCC) for a 500-test sample dataset yields an accuracy of 55.9%, emphasizing the struggle
215 of the ASNN to precisely predicting resonant features of the S_{11} parameters with this data format.

216 To overcome this struggle, we transform the spectral data to an image-like data format that is more
217 suitable for CNNs. Specifically, our approach involves directly extracting the contour of the reflection
218 spectrum and resizing this information into 100 x 100 images, as depicted in Fig. 3a. Harnessing the
219 intrinsic advantages of CNNs in the domain of image processing, we represent the S_{11} parameters
220 as image inputs, allowing the CNN to efficiently process two-dimensional image data. This method
221 yields a data format from which the CNN-based ASNN can extract more relevant abstract features (Fig.
222 3c). Importantly, this simple data reformatting process facilitates the learning of relevant features
223 from extensive datasets, eliminating the need for intricate and computationally intensive feature
224 extraction procedures.

225 **Training results and comparison with conventional neural networks.** We utilize a total of 5,000
226 samples generated by CST studio suite for normally incident electromagnetic waves in order to train
227 INN 1/2 and ASNN. The very large targeted frequency range is 6-13 GHz. The samples are randomly
228 divided into training, validation, and testing sets at an 8:1:1 ratio. The training results for INNs and
229 ASNN are illustrated in Figs. 4a and 4c, indicating satisfactory validation losses compared to the
230 training losses. The predictions for three arbitrarily selected samples from the test set are depicted in

231 Figs. 4b and 4d, where the actual and predicted S_{11} images exhibit remarkable similarity, even in the
232 vicinity of sharp spectral features. To quantify the training effectiveness, we employ the structural
233 similarity index (SSIM) as a metric, widely recognized in image processing to assess similarity across
234 luminance, contrast, and structure. Calculating SSIM for the entire test dataset, we obtain results of
235 98.4% and 99.7% for INN 1/2, and 96.7% for ASNN, providing further quantitative evidence of the
236 robust generalization capabilities of our synthetic neural network.

237 **Scalability of synthetic neural network.** To further illustrate the adaptable assembly feature and
238 recyclable nature of our network, we embedded an annular ring, R_{14}^{10} , within the design of R_{10} (Fig.
239 5a). For this new R_{14} design task, data from the previous R_8 and R_{10}^8 , along with the networks
240 (INN1/2), could be leveraged. Rebuilding and training the R_{14}^{10} network, akin to R_{10}^8 , and introducing
241 a new ASNN' were the only requirements. The training outcomes of INN3 with 5,000 examples for
242 R_{14}^{10} and the new ASNN' are depicted in Figs. 5b and 5d, achieving high SSIM values of 99.2% and
243 95.5%, respectively. The predictions for random samples from the test set are displayed in Figs. 5c
244 and 5e, emphasizing our network's remarkable recyclability in efficiently utilizing resources while
245 consistently delivering high-quality results, and significant knowledge-inheritance capabilities when
246 applied to a new task.

247 For comparative analysis, we perform the R_{14} design task with the same amount of training data
248 using a CNN, sharing a structure akin to the INN (i.e., featuring both inverse and forward modules).
249 The training results, illustrated in Fig. 5f, reveal an inability of the CNN to converge, showcasing a
250 pronounced underfitting condition with an accuracy of only 70.5%. This substantial underfitting
251 becomes notably evident when examining the S_{11} outcomes for the three test samples in Fig. 5g.
252 The stark inconsistency in results strongly affirms that the CNN is ineffective when exposed to the
253 same training data. This benchmarking further underscores the superiority and efficiency of our
254 synthetic neural network over traditional "indivisible" design methods.

255 Discussion

256 In conclusion, we have introduced the modular broadband synthesis of neural networks for
257 metasurface inverse design that inherits and efficiently combines knowledge from multiple neural
258 networks previously trained on related sub-tasks. Our approach speeds up the metasurface design
259 process by efficiently integrating prior insights and experiences, akin to the genetic inheritance

260 through generations. Thereby, both the amount of required training data and the required
261 computational resources and compute time can be significantly reduced, such that our approach
262 economizes scarce resources in an environmentally sustainable manner. The proposed low-cost
263 design methodology reduces redundant computations and expedites the design process. Our work
264 demonstrates great adaptability and scalability and, importantly, manages to accurately capture
265 sharp resonant features and intricate coupling effects between metasurface segments. Additionally,
266 the proposed data formatting eliminates the challenges posed by spectral data for CNN-based
267 networks. Looking forward, we anticipate the widespread integration and proliferation of our
268 approach in the field of material science.

269 **Materials and methods**

270 **Data generation and training details.** The reflection spectrum data of different metasurfaces is
271 generated through CST studio suite, with the incident wave perpendicular at a position 30mm away
272 from the metasurface. In this way, we first generate 5,000 datasets of each “parent” component by
273 randomly setting the metasurface distribution for INN training. Then, for an “offspring” metasurface
274 (assembled by “parent” components), we also follow the similar procedure to generate 5,000
275 samples for ASNN training. The Adam optimizer⁴⁵ is employed to update the parameters to complete
276 the training of the models. During training, the epochs and batch size of the INN are set to 100 and
277 64, and those of the ASNN are set to 100 and 128, respectively. The initial learning rates of the INN
278 and the ASNN are both 0.0001, which will continue to shrink by a ratio of 0.5 when the validation loss
279 stops improving, and the update is terminated when the minimum learning rate of 10^{-5} is reached.
280 In this way, the optimal model can be obtained quickly and accurately. For the ASNN, the loss function

281 MSE is formally expressed as $MSE = \frac{1}{P*Q} \sum_{i=1}^P \sum_{j=1}^Q (S_{ij} - S_{ij}')^2$, where $S_{ij}(S_{ij}')$ denotes the j th
282 sampling point of the ground-truth (predicted) S_{11} image pertaining to the i th reflection spectrum.
283 Here, P assumes a value of 4, with odd indices representing $\text{Re}(S_{11})$ and even indices
284 corresponding to $\text{Im}(S_{11})$. The variable Q denotes the 100 x 100 S_{11} images.

285 **Deep learning architecture.** The INN is divided into two modules, i.e., a CNN module for the inverse
286 design and a forward module for the forward mapping. For the CNN module, there are 7 convolution
287 layers and 3 deconvolution layers, in which the seventh layer are used for fusing the processed
288 features and further exporting the metasurface design \mathbf{R} which is binarized to comply with the
289 physical design constraint. A sigmoid function is applied to the final layer of the forward network to
290 ensure the output falls within the [0, 1] range. The layers are followed by batch normalization and
291 rectified linear unit (ReLU) layers. The inclusion of batch normalization and ReLU layers expedites the
292 training process and bolsters the network's robustness, effectively mitigating challenges associated
293 with vanishing gradients and overfitting. All models are trained on a CPU of Intel (R) Core (TM) i7-
294 8700K and a graphics processing unit (GPU) of NVIDIA GeForce RTX 2080 SUPER.

295

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303 **Conflict of interest**

304 The authors declare no competing financial interests.

305 **Contributions**

306 C.Q., Y.J., and H.C. conceived the idea. Y.J. performed the simulation and machine learning part. Z.F.
307 provided assistance with the machine learning. Y.J. and C.Q. wrote the paper. P.d.H. contributed to
308 the discussion of the results and writing of the paper. C.Q. and H.C. supervised the project.

309 **Data availability**

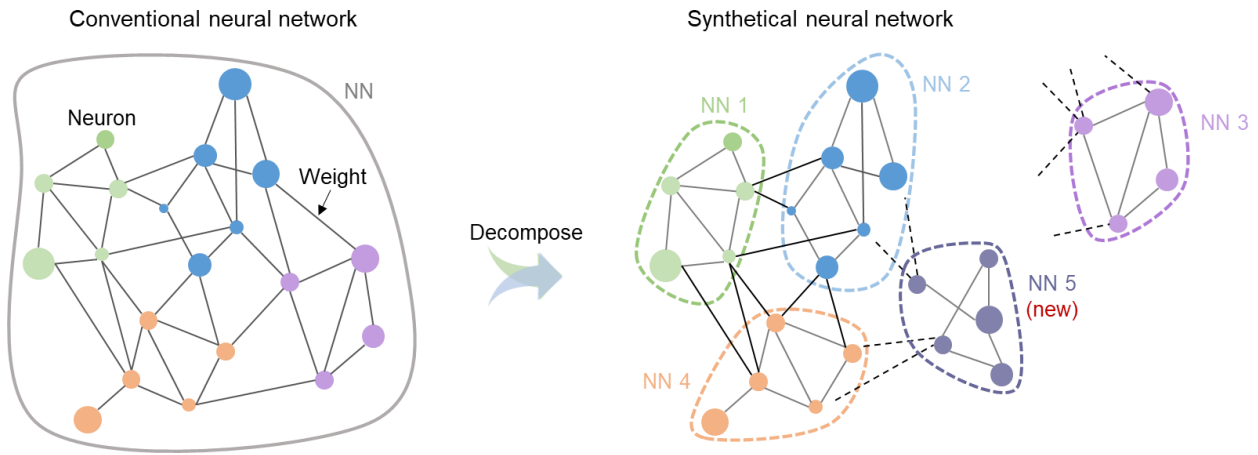
310 The data that support the findings of this study are available from the authors on reasonable request.

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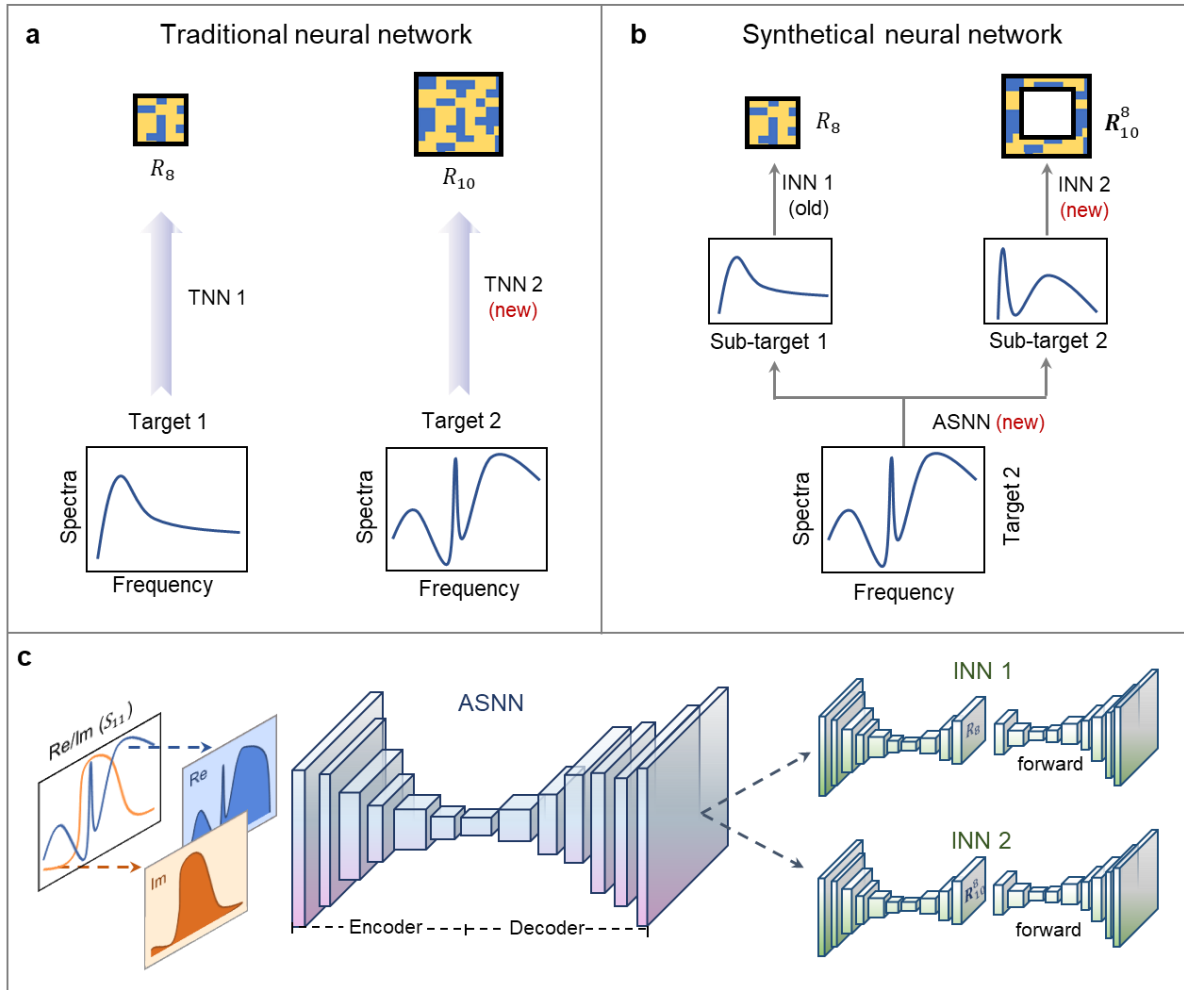
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400 **Fig. 1 | Comparison of conventional and synthetical neural network.** Neural networks, emulating
 401 the biological nervous system, consist of interconnected neurons that process input through
 402 weighted mechanisms to generate the output. In conventional neural networks, the network is
 403 typically indivisible and necessitates an abundance of data for training. Our synthetical neural
 404 network shifts this paradigm by breaking down the solution space. Each subproblem is assigned to a
 405 specific neural network (e.g., NN 1~NN 4). These neural networks can be freely assembled to adapt
 406 to different tasks. When faced with a completely new task, selecting appropriate NNs and assembling
 407 them in a specific order allows for the swift synthesis of an entirely new network, as illustrated by
 408 the free assembly of NN 1/2/4 and the newly added NN 5.

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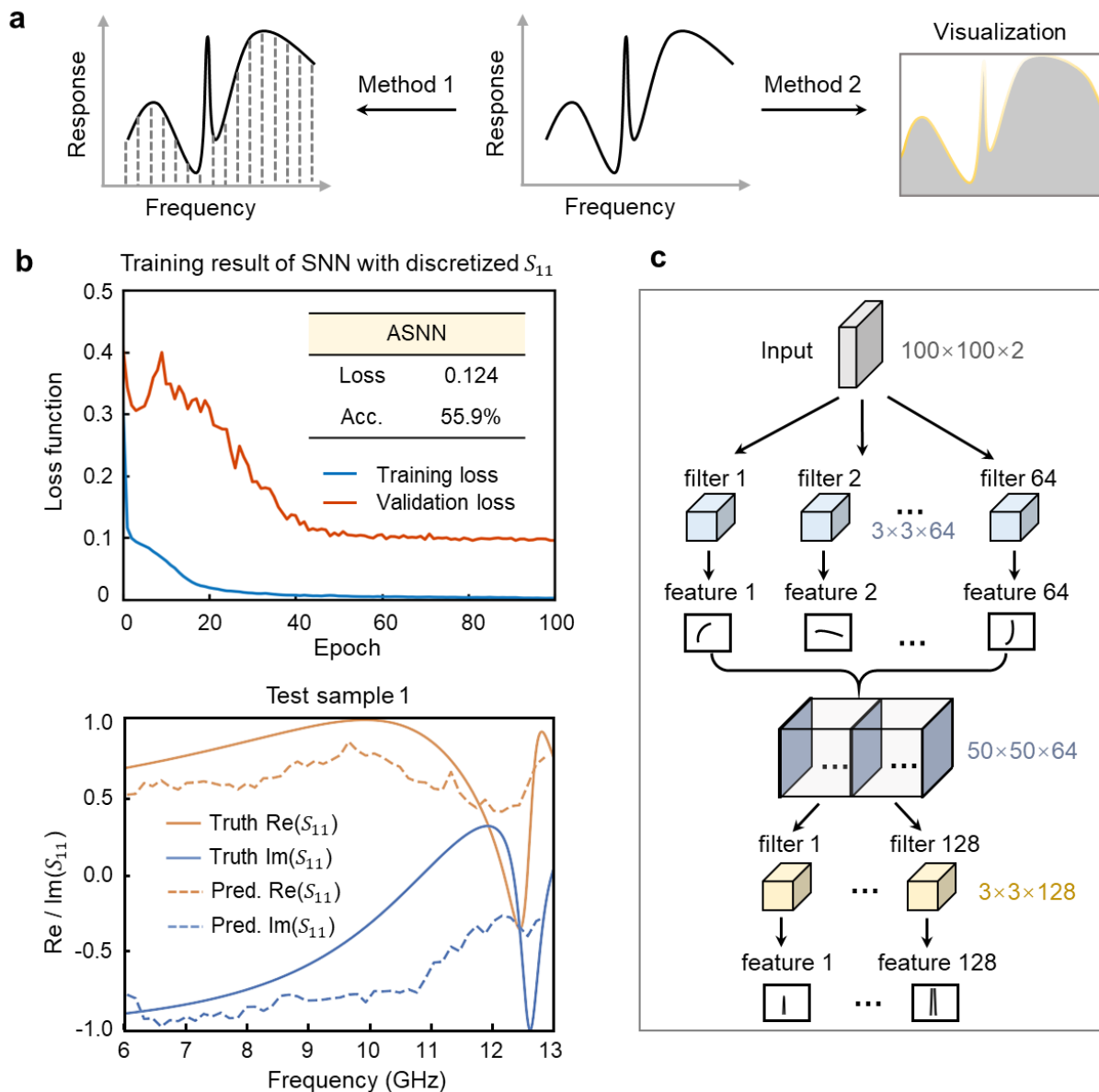
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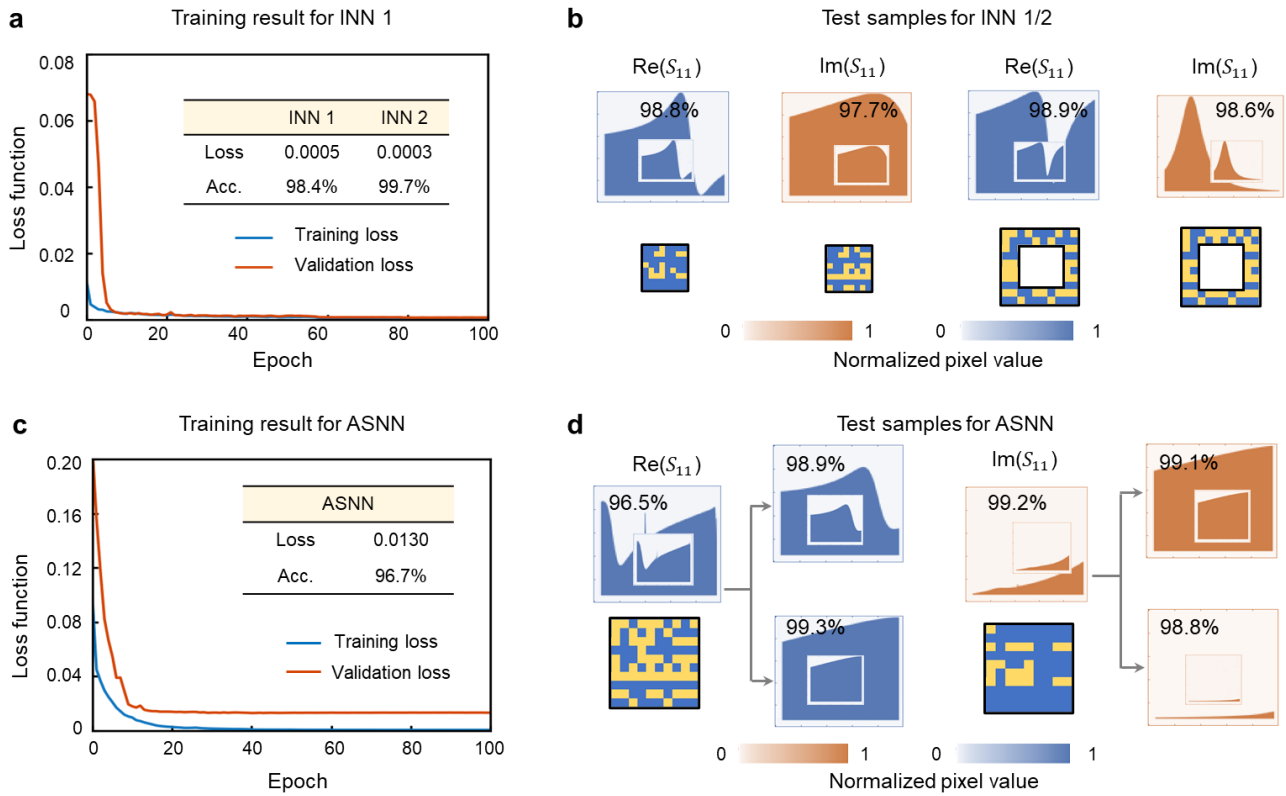
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Fig. 2 | Design and architecture of the synthetical neural network. **a**, In metasurface inverse design, the conventional methodology involves utilizing the reflection spectrum (S_{11} parameter) as the input and obtaining the metallic resonant surface as the output through machine learning-based optimization. In the conventional method, the task-specific neural network (TNN 1) must be discarded when transitioning to a new task (Target 2) with a new required TNN 2, presenting a time-consuming challenge. **b**, Our method treats metasurfaces as composite structures assembled from different "parent" segments. Each segment has an associated inverse design network (INN), systematically cataloged in a "gene" library. When confronted with a new task (Target 2), we assemble the pre-trained INN1 (old) and the INN2 (new) corresponding to R_{10}^8 using the ASNN. This assembly method mitigates data requirements to a certain extent, and each newly added INN can be stored in the gene library for future reuse. **c**, The INN and ASNN are structured as CNNs with an encoder-decoder configuration, where the input/output consists of compressed S_{11} images (including real and imaginary parts) as detailed in Fig. 3. The forward design networks included in the INN addresses the non-uniqueness challenge of inverse design.



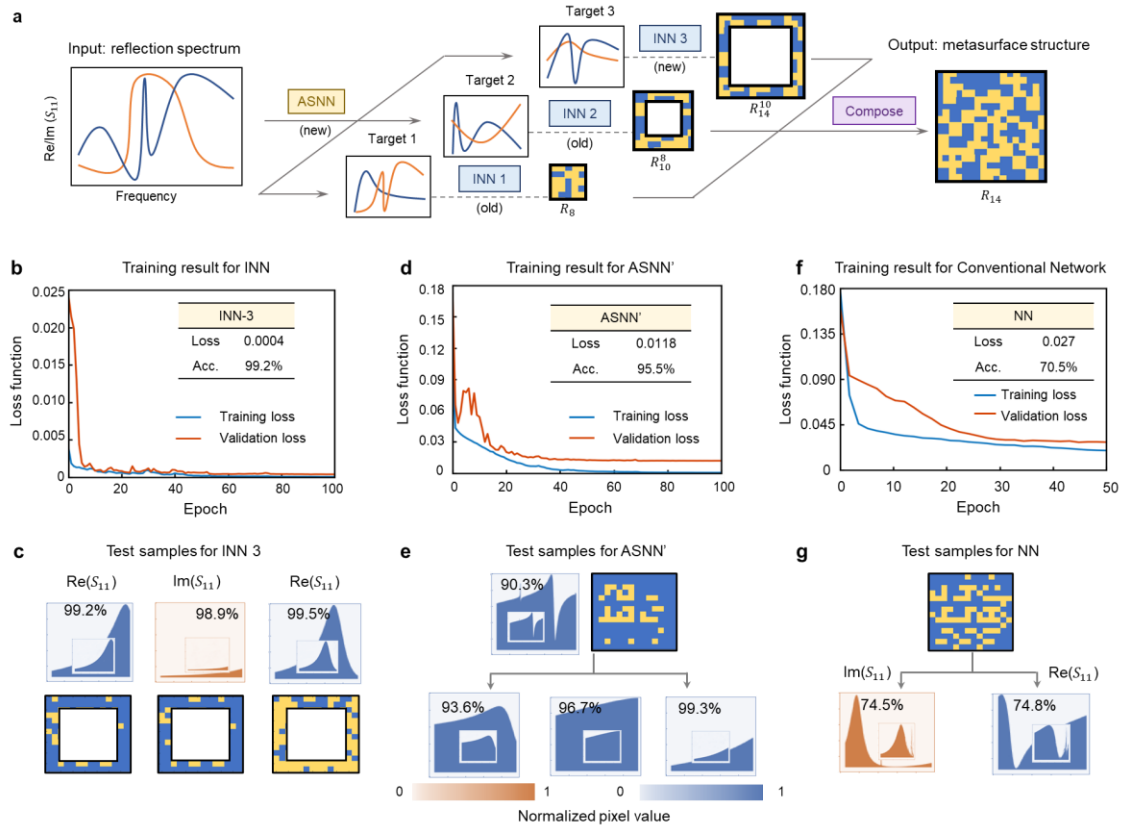
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426 **Fig. 3 | Pre-processing of spectral data.** **a**, Two distinct processing methods for spectral data. Method
 427 1 is a simple 1D discretized representation of the continuous physical spectrum. Method 2 formats
 428 the representation from Method 1 into a 100 x 100 image. **b**, Results of ASNN training with Method
 429 1. The network only achieves an accuracy of 55.9%. Examining Test sample 1 to observe the training
 430 effect, the notable discrepancy between predicted (dotted line) and actual values (solid line) further
 431 illustrates the suboptimal outcome of the training. **c**, Illustration of the CNN-based encoder. Method
 432 2 is more suitable for CNN-based image processing. Through convolution/deconvolution operations
 433 on local pixel information, the network gradually aggregates the knowledge of sharp resonant
 434 features at higher layers.



435

436 **Fig. 4 | Training results for INN/ASNN.** **a**, Training results for INN 1 over training epochs, reaching an
 437 accuracy of 99.4%. The accuracy for INN 2 is 99.7%. **b**, Predicted real/imaginary S_{11} images of four
 438 samples by INN 1/2, with embedded insets depicting the corresponding ground-truth images. The
 439 close correspondence between the ground-truth images and the predicted images highlights the high
 440 accuracy. The corresponding R_8/R_{10}^8 patterns of the predicted metasurface are displayed below. **c**,
 441 Training results for the ASNN over the training epochs, reaching an accuracy of 96.7%. **d**, Predicted
 442 real (blue)/imaginary (yellow) S_{11} images of R_{10} by the synthetical neural network, with
 443 embedded insets depicting the ground truth image and the accuracy. The predicted R_{10} patterns
 444 are displayed below. The corresponding split S_{11} images of the two “parent” components (R_8/R_{10}^8)
 445 are connected by arrows.



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447 **Fig. 5 | Scalability of synthetic neural network.** **a**, For the new R_{14} design task, there is no need
 448 to collect and train new data and networks specific to R_{14} . The process involves reusing two existing
 449 INNs, namely INN 1 and INN 2, based on the framework depicted in Fig. 2a. However, the introduction
 450 of a new INN 3, dedicated to INN 3 to the R_{14}^{10} annular ring, is necessary. Subsequently, a new ASNN' to
 451 assemble all three INNs is trained to accomplish the inverse design task for R_{14} . **b**, Training results
 452 for INN 3 over the training epochs, reaching an accuracy of 99.7%. The blue and red lines represent
 453 the training and validation losses, respectively. **c**, Predicted real/imaginary S_{11} images of three
 454 samples with INN 3 for the new R_{14}^{10} "parent" component, with embedded insets depicting the
 455 ground-truth image; the achieved accuracies are stated. The predicted R_{14}^{10} "parent" components
 456 are displayed below. **d**, Training results for the new ASNN' over the training epochs, reaching an
 457 accuracy of 95.5%. **e**, Predicted real S_{11} images of one sample by the new synthetic neural network,
 458 with embedded insets depicting the ground-truth image. On the right side, the corresponding
 459 predicted "parent" component, R_{14} , is displayed. Arrows connect the corresponding split S_{11}
 460 images of $R_8/R_{10}^8/R_{14}^{10}$. **f**, Training results for the conventional neural network over the training
 461 epochs. It is in a serious underfitting state, and its accuracy is only 70.5%. **g**, Predicted real/ imaginary
 462 S_{11} images by conventional network.