Optimal Design: Old and New

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Contents

Standard approaches

A toy example: Minimum compliance design[1]:

$$\min_{\mathbf{u}\in\mathbf{U},\mathbf{E}} l(\mathbf{u}) = \int_{\Omega} \mathbf{f}^{\top}\mathbf{u}\mathrm{d}\Omega + \int_{S_\sigma} \mathbf{t}^{\top}\mathbf{u}\mathrm{d}S \tag{1}$$

subject to

$$\begin{aligned} a(\mathbf{u},\mathbf{v}) = \int_{\Omega} E_{ijkl}\varepsilon_{ij}\varepsilon_{kl}\mathrm{d}\Omega = l(\mathbf{v}), \quad \forall \mathbf{v} \in \mathbf{U}, \\ \mathbf{E} \in \mathbf{E}_{\mathrm{ad}}. \end{aligned} \tag{2}$$

- Solid Isotropic Material Penalization (SIMP)
- Homogenization
- Level set method

[1] MP Bendsøe and O Sigmund. *Topology Optimization. Theory, Methods, and Applications*. 2nd ed. Berlin Heidelberg: Springer-Verlag, 2004.

Problem description

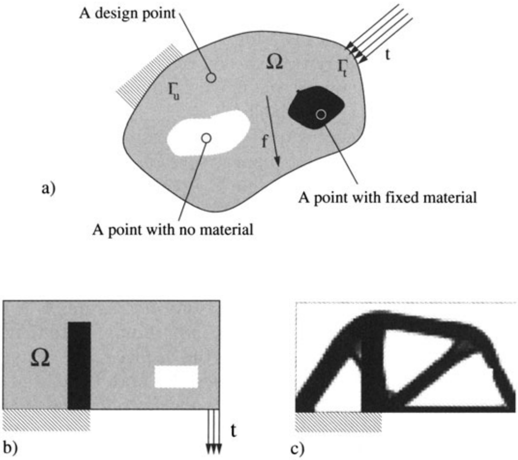


Figure: A minimum compliance problem. Reprinted from [1].

Discrete formulation

$$\min_{\mathbf{u}_h, \mathbf{E}_e} \mathbf{f}^\top \mathbf{u}_h \tag{3}$$

such that

$$\begin{aligned} \sum \mathbf{K}_e(\mathbf{E}_e)\mathbf{u}_h &= \mathbf{f}, \\ \mathbf{E}_e &= 1_{\Omega^*}\mathbf{E}^0, \\ \int_\Omega 1_{\Omega^*} \mathrm{d}\Omega &\leq V. \end{aligned} \tag{4}$$

This integer programming problem is very hard to solve.

SIMP

$$\mathbf{E}(\mathbf{x}) = \rho(\mathbf{x})^p \mathbf{E}^0, \quad \text{with } p > 1, \tag{5}$$

subject to

$$\rho(\mathbf{x}) \in [0,1] \text{ and } \int_\Omega \rho \mathrm{d}\Omega \leq V. \tag{6}$$

For large p, e.g. $p \geq 3$ in 2D, the existence of a global 0-1 solution (to the discrete problem) was proved under mild assumptions[2]. The exponent p can also be regarded as a "real" material parameter.

Optimality criteria? Sensitivity analysis? Can the discrete solution well approximate the continuous solution?

[2] A Rietz. "Sufficiency of a finite exponent in SIMP (power law) methods". *Structural and Multidisciplinary Optimization* 21 (2001), 159–163.

Issues of SIMP I

Mesh-dependent solutions & Checkerboard pattern

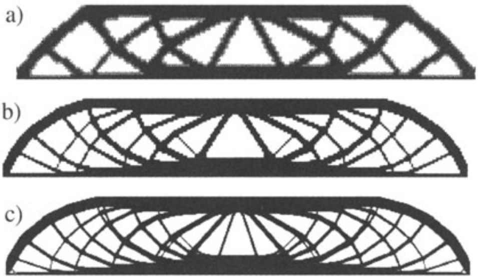


Figure: Mesh-dependent solutions of a three-point bending problem. Reprinted from [1].

Issues of SIMP II

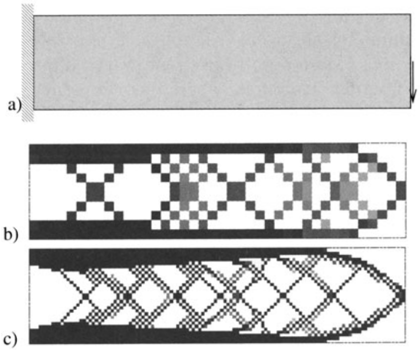


Figure: The checkerboard problem. Reprinted from [1].

Solutions: Constraining the gradient of ρ. Adding filters.

Homogenization

Shape/topology optimization ≈ Finding the optimal composite (composed of void and the original material)

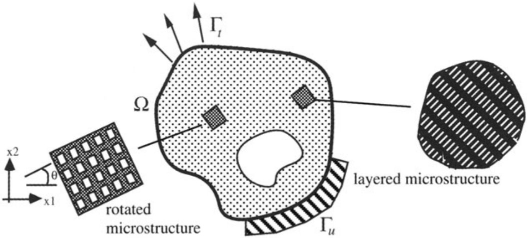


Figure: Material with microstructure. Reprinted from [1].

Homogenization formulation

The structure is made of (infinitely many) periodically distributed (infinitely small) cells (with size δ). What happens if $\delta \to 0$?

We again minimize the compliance subject to:
$a(\mathbf{u}, \mathbf{v}) = l(\mathbf{v}),\ \forall \mathbf{v} \in \mathbf{U}$,
geometric variables $\mu,\ \gamma,\ \cdots \in L^\infty(\Omega)$, angles $\theta \in L^\infty(\Omega)$,
$\mathbf{E} = \tilde{\mathbf{E}}(\mu, \gamma, \ldots, \theta)$,
density ρ is a function of these parameters,
and $\int_\Omega \rho(\mathbf{x}) \leq V$ with $0 \leq \rho \leq 1$.

How to enforce 0-1 solution? (Penalization)

Level set method

Represent the shape using a level set function ϕ, and explicitly using the shape sensitivity to perform gradient descent[3].

Define a perturbed domain by $\Omega^*_\theta = (\mathrm{Id} + \theta)(\Omega^*)$, where θ is a small vector field.

Denote $J(\Omega^*)$ the objective function. It can be shown

$$J'(\Omega^*)(\theta) = \int_{\partial\Omega^*} v(J)\theta \cdot \mathbf{n} \mathrm{d}\Omega. \tag{7}$$

Now $\theta = -v\mathbf{n}$ is a descending direction. The level set function is updated by

$$\frac{\partial \phi}{\partial t} - v\|\nabla \phi\| = 0. \tag{8}$$

[3] G Allaire, F Jouve, and AM Toader. "Structural optimization using sensitivity analysis and a level-set method". *Journal of Computational Physics* 194.1 (2004), 363–393.

Machine learning–based approaches I

Topology optimization of 2D nonlinear structures[4].

“HPC cluster” at National Center for Supercomputing Applications (NCSA) + “Commercial FEA software ABAQUS” + “SIMP” + “Simple CNN”.

Direct learning of the optimal configuration given loading and constraints. 15000 data generated at a speed of 0.31 min/data point (linear) or 3.2 min/data point (nonlinear, and with 10 parallel instances).

[4] DW Abueidda, S Koric, and NA Sobh. “Topology optimization of 2D structures with nonlinearities using deep learning”. *Computers & Structures* 237 (2020), 106283.

Machine learning–based approaches I

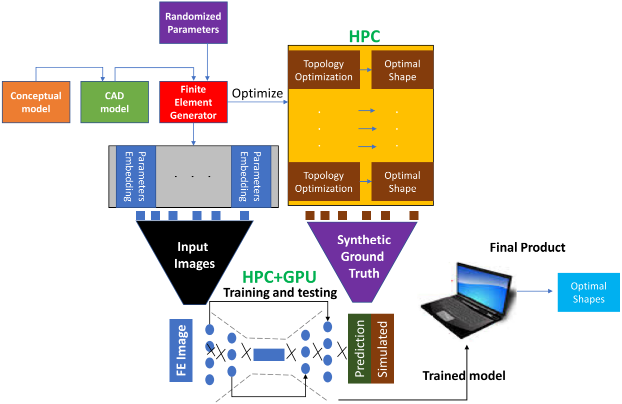


Figure: A training flowchart. Reprinted from [4].

Machine learning–based approaches I

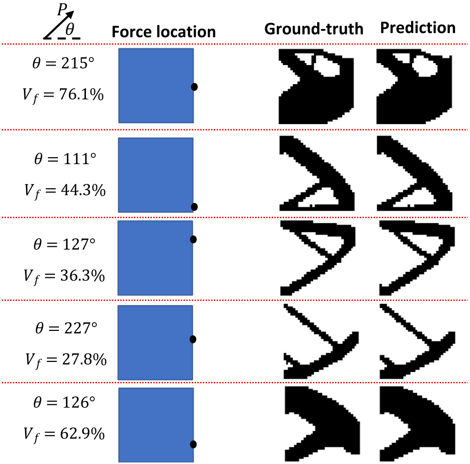


Figure: Performance of the CNN optimizer. Reprinted from [4].

Machine learning–based approaches II

Aerodynamic design optimization (max lift-to-drag ratio) using GANs[5].

"Dimensionality reduction infoGANs" + "Real shape data UIUC airfoil database" + "Interactive solver XFOIL" + "Mixed optimization".

[5] W Chen, K Chiu, and M Fuge. "Aerodynamic design optimization and shape exploration using generative adversarial networks". In: *AIAA Scitech 2019 Forum*. San Diego, California: AIAA, 2019.

Machine learning–based approaches II

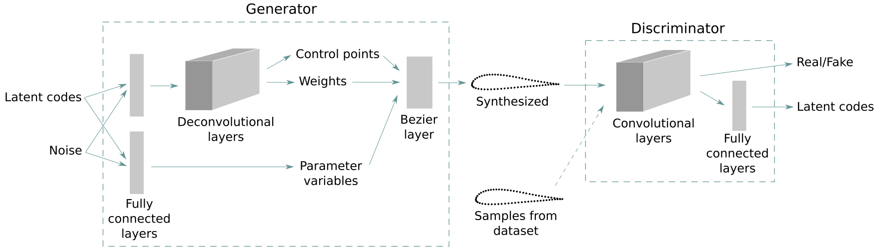


Figure: The infoGAN for dimensionality reduction. Reprinted from [5].

Machine learning–based approaches II

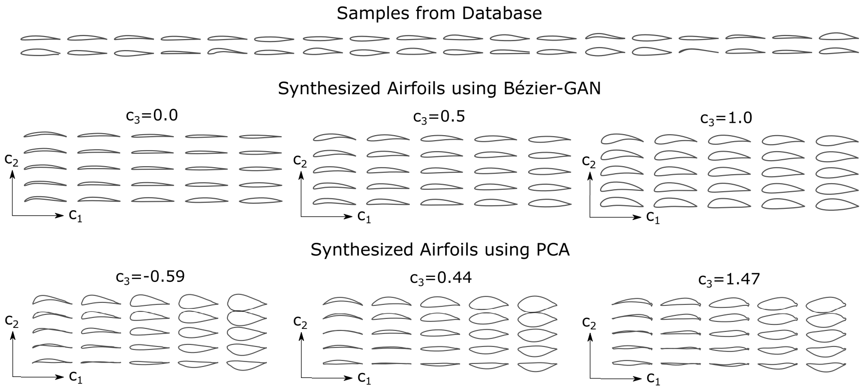


Figure: The latent space of infoGAN. Reprinted from [5].

Machine learning–based approaches II

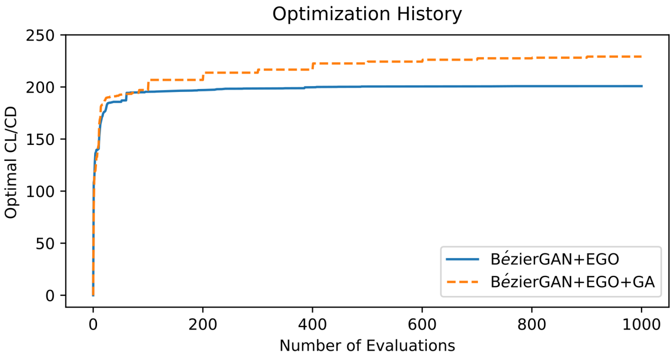


Figure: Performance of the mixed optimization approach. Reprinted from [5].

Tasks

- Predicting the properties of a given composite.
  - Simple assumptions. (inaccurate)
  - Curve fitting based on experimental measurements or numerical simulations. (1D)
  - ...
- Multiscale modeling.
- Optimal design.

Constitutive models

- Simple models: linear elasticity, perfect plasticity, ... (1D)
- Mass conservation + momentum conservation + energy conservation + Entropy imbalance + frame-indifference. (3D theoretical models)
- Real materials???

Use CNN or RNN to learn from real data. How to obtain $\{(\varepsilon_i, \sigma_i)\}$ from experimental tests? How to learn 3D constitutive models? How to use such trained models with FEA? Efficiency?

Multiscale modeling

Representative volume element[6] forms the basis for many multiscale analysis methods[7], in which the local mechanical properties of a composite structure are approximated by the response of a representative micro structure.

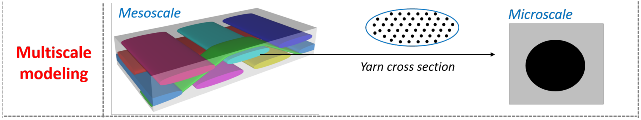


Figure: Micro structure at a material point. Reprinted from [7].

[6] CT Sun and RS Vaidya. "Prediction of composite properties from a representative volume element". *Composites Science and Technology* 56.2 (1996), 171–179.

[7] X Liu et al. *How machine learning can help the design and analysis of composite materials and structures?* 2020. arXiv: 2010.09438 [cond-mat.mtrl-sci].

Homogenized material properties

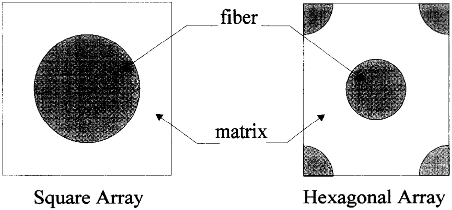


Figure: Two typical representative volume elements. Reprinted from [6].

$$\bar{\sigma}_{ij} = \frac{1}{V}\int_V \sigma_{ij}\mathrm{d}V,\ \bar{\varepsilon}_{ij} = \frac{1}{V}\int_V \varepsilon_{ij}\mathrm{d}V, \\ \bar{\sigma}_{ij} = E_{ijkl}\bar{\varepsilon}_{kl}. \tag{9}$$

Computational cost: $O(N_{\mathrm{quad}}N_{\mathrm{ele}}N_{\mathrm{iter}})$ FE simulations. Directly modeling the mapping $f(\mathrm{input}) = \mathrm{output}$ can dramatically reduce the cost.

Design a composite structure

Without NN-based surrogate models, design of a composite structure typically requires numerous sequential analyses of the parameterized problem[8].

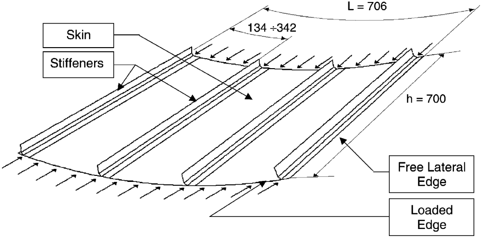


Figure: Composite stiffened panel. Reprinted from [8].

[8] C Bisagni and L Lanzi. "Post-buckling optimisation of composite stiffened panels using neural networks". *Composite Structures* 58.2 (2002), 237–247.

Details of the training process

Learned mapping: design parameters $\rightarrow$ loading-displacement curve.
Optimization method: Genetic algorithm.
Dataset: **70 eigenvalue analyses and 55 dynamic analyses (took about 660 hours on a parallel machine)**.
Training + optimization time: **about the cost of a single FE simulation**.
Direct optimization took near 9480 hours.

Tasks

- Forward design: Given a sub-scale structure, compute the optical response by solving Maxwell's equations. (easy)
- Inverse design: Find a proper structure that yields the desired response. (challenging) Traditional optimization approaches require solving the forward problems many times in a sequence.

Structure topology optimization $\approx$ inverse design in photonics.

Two NN-based approaches: Training a surrogate model to approximate the forward calculation, or directly learning the inverse mapping using NNs[9,10].

[9] W Ma et al. "Deep learning for the design of photonic structures". *Nature Photonics* 5 (2021), 77–90.

[10] PR Wiecha et al. "Deep learning in nano-photonics: inverse design and beyond". *Photonics Research* 9.5 (2021), B182–B200.

The one to many issue

The inverse design problem usually has multiple solutions. An example is given below[11].

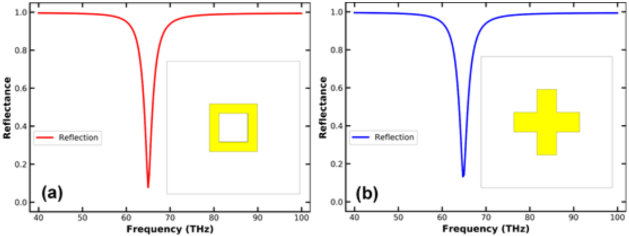


Figure: Two designs with the same response. Reprinted from the supplemental material of [11].

[11] W Ma et al. "Probabilistic representation and inverse design of metamaterials based on a deep generative model with semi-supervised learning strategy". *Advanced Materials* 31.35 (2019), 1901111.

How to learn a one-to-many mapping?

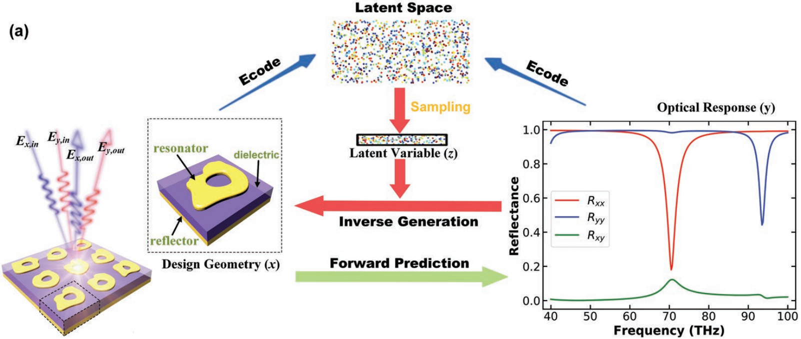
Naive FCNN can only learn an averaged mapping. (large error)

Solutions:

- Tandem training method.
- Dimensionality reduction using autoencoders[12].
- Conditional GANs and VAEs.

[12] Y Kiarashinejad, S Abdollahramezani, and A Adibi. "Deep learning approach based on dimensionality reduction for designing electromagnetic nanostructures". *npj Computational Materials* 6.12 (2020), 1–12.

A VAE example I



A VAE example II

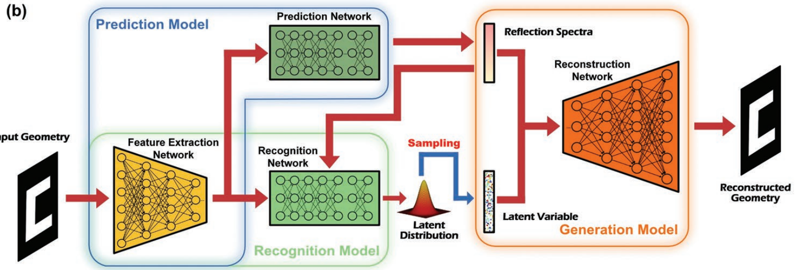


Figure: A conditional VAE model for photonics design. Reprinted from [11].

- Obtaining data efficiently.
- Benchmark problems for performance testing.

Thank you.

References I

- Abueidda, DW, S Koric, and NA Sobh. "Topology optimization of 2D structures with nonlinearities using deep learning". *Computers & Structures* 237 (2020), 106283.
- Allaire, G, F Jouve, and AM Toader. "Structural optimization using sensitivity analysis and a level-set method". *Journal of Computational Physics* 194.1 (2004), 363–393.
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References II

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References III

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