



Optimization of an Optical Shutter using Machine Learning

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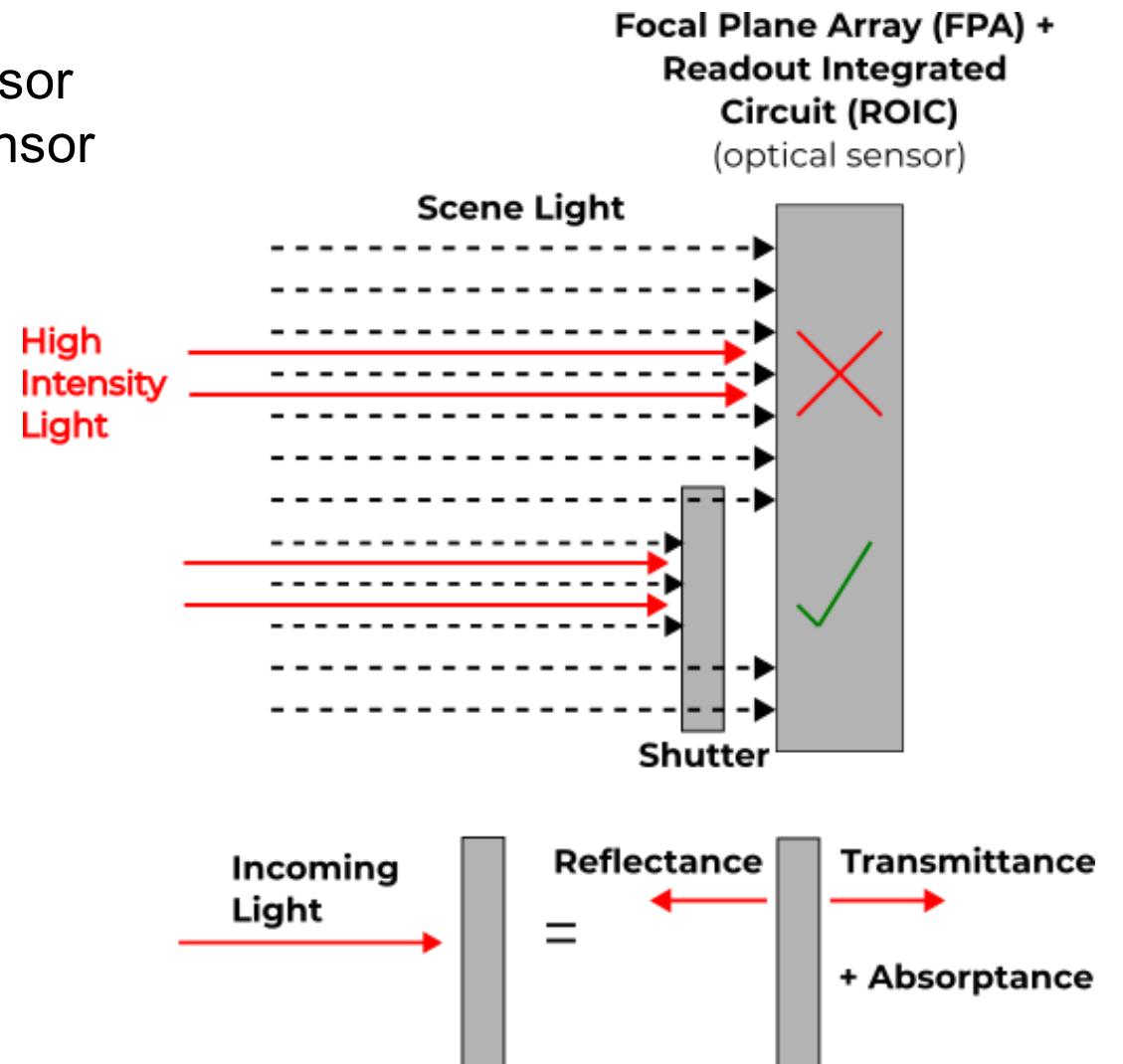
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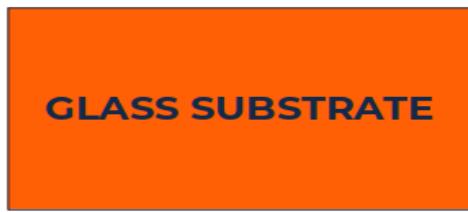
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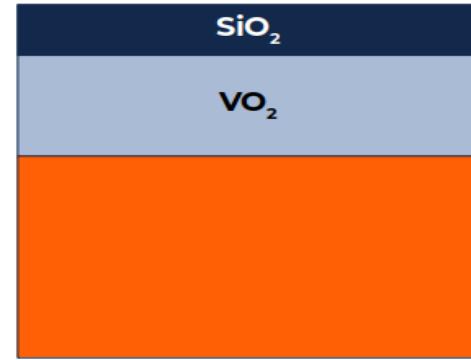


- **Purpose:** sensor protection using optical shutter
 - Normal operation: scene light reaches optical sensor
 - High intensity light: can overwhelm or damage sensor
- **Ideal scenario:** passively switch the shutter on and block/reflect the high intensity light
- Utilize VO_2 :
 - Phase change material: thermally triggered
 - Insulating (monoclinic) phase: low-loss, semi-transparent
 - Metallic (rutile) phase: lossy, reflective
- Figures of merit
 - **Extinction ratio:**
 - Transmittance on / Transmittance off
 - Bigger is better
 - **Temperature rise:**
 - Efficiently switch on
 - Bigger is better

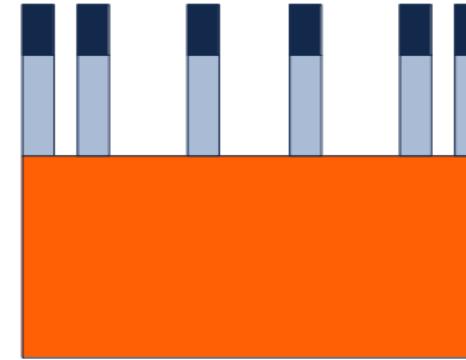




No Film
Low insertion
Low extinction
No temp rise



Full Film
High Insertion
High extinction
Avg temp rise



Interm. insertion
Interm. extinction
Temp rise?

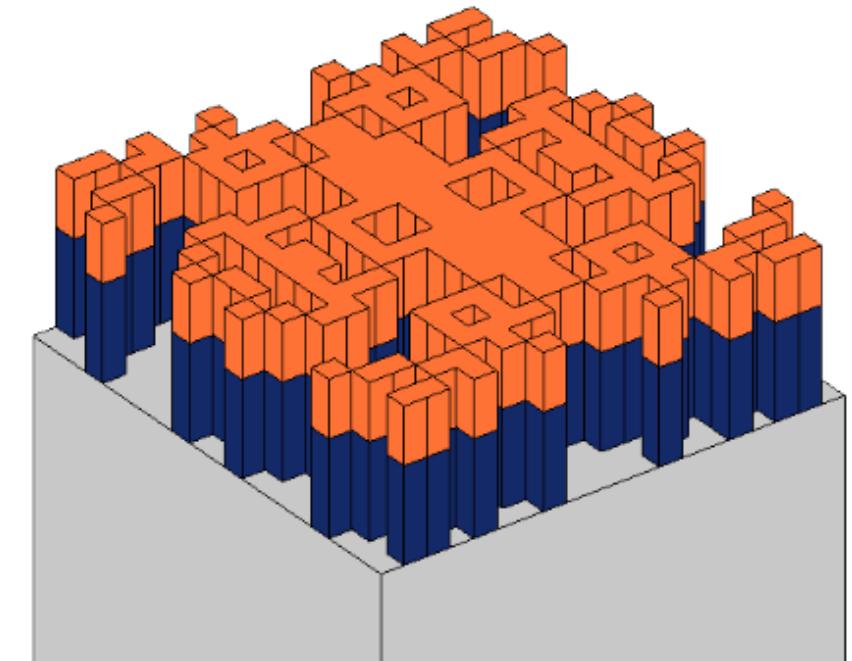


$$\text{Ext ratio} = 10 \log_{10} \frac{T_{rins}}{T_{rmet}}$$

Can we find a pixelated design that maximizes temperature rise for a given extinction ratio?

Topology Optimization

- **Goal:** Optimization of optical switch using phase change material (VO_2) using machine learning
- **Plan:**
 - Perform simple modeling to generate data
 - Optimize using a completely machine learning (ML) approach
 - Check using FEA
 - Fabricate/test at Sandia National Lab



Approach - Traditional Topology Optimization



- Discretize problem:
 - Write governing equation, set boundary conditions, discretize domain
 - Finite element setup
- Allocate a given amount of material across the points
 - Density function (ρ)
 - $\rho = 0$ means no material, 1 means material
 - Discrete = Tough
 - Use continuous
- Determine objective (cost) function to minimize; e.g. compliance (structural) or band gap (EM)
 - In our case, extinction ratio and temperature rise targets
- Iterate, determine gradient, adjust, repeat
 - **Requires costly finite element solver calls each iteration**

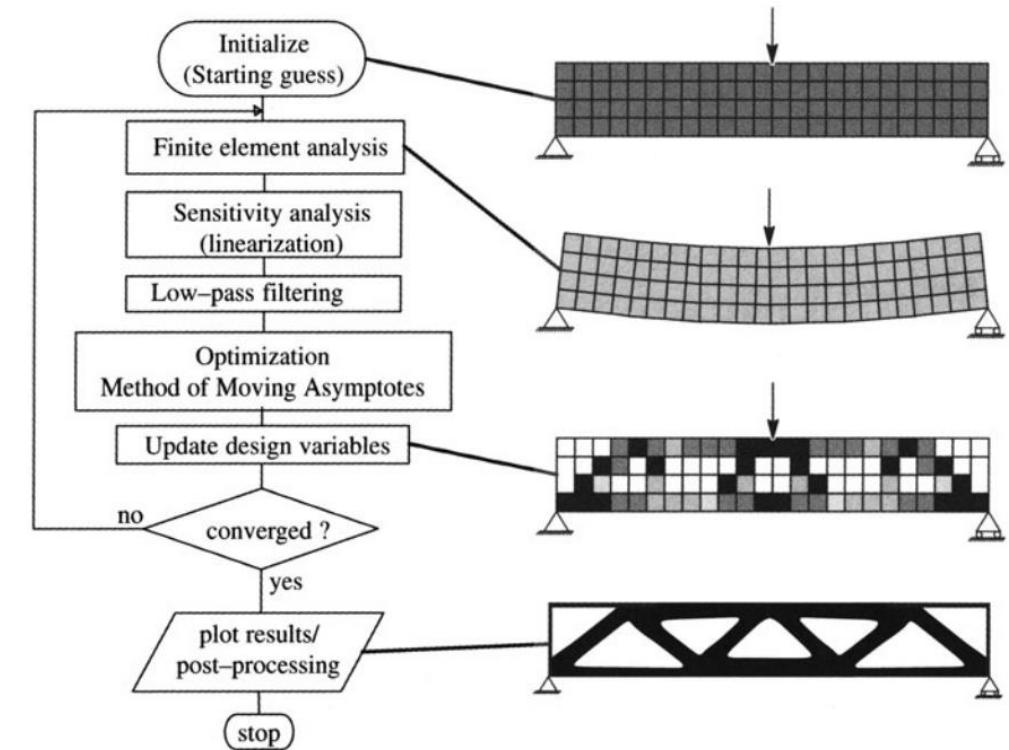


Fig. 1.5. The flow of computations for topology design using the material distribution method and the Method of Moving Asymptotes (MMA) for optimization. The low-pass filter step (filtering of sensitivities) is discussed in Sec. 1.3.1.

Source: Bendsøe and Sigmund, "Topology Optimization: Theory, Methods, and Applications", 2003

Optimization using ML



- Neural Networks (NNs) for topology optimization:
 - Collection of variables that get changed to perform a task
 - Image classification, regression, etc.
 - Allow for accurate and cheap prediction of device performance
 - Can be trained to provide design performance (FEA) and density function (material distribution)
- Utilize Convolutional Neural Networks (CNNs) to bypass COMSOL model after training (Performance Neural Network - PerfNet)
 - Heavily used for image recognition
 - Scanning an image, looking for patterns
 - Excels at image/pattern recognition
 - Dot product between kernel (filter) and feature combine to create feature map
- Utilizing Pytorch, an open source ML package
- Train model using labeled data (supervised model)

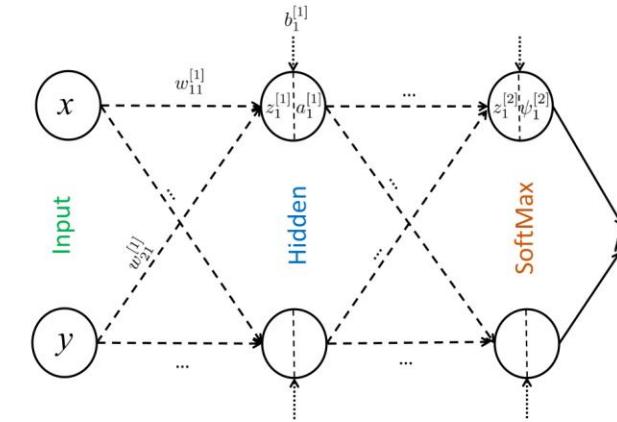
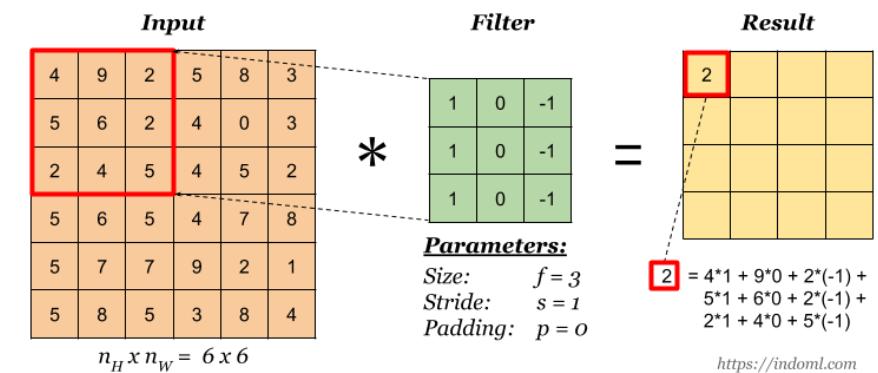


Fig. 4 Illustration of a simple network with one hidden layer of height 2

Source: Chandrasekhar and Suresh, "TOuNN: Topology Optimization using Neural Networks," <https://doi.org/10.1007/s00158-020-02748-4>

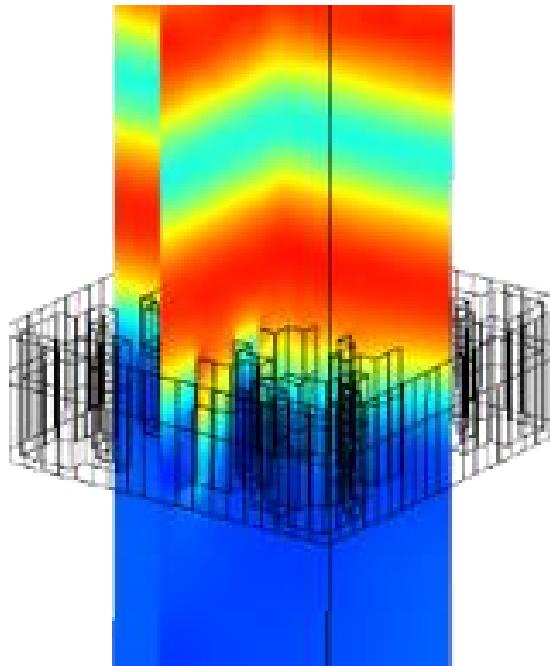


Source: <https://medium.com/analytics-vidhya/everything-you-need-to-know-about-convolutional-neural-networks-cnns-3a82f7aa29c5>

Generating Training Data with COMSOL



- Generate designs (symmetric about x and y axis)
- Run frequency domain model in insulating phase:
 - Tr_{ins}
- Using insulating absorptance (total power dissipation density), run time domain model:
 - **Temp rise**
- Run frequency domain model in metallic phase:
 - Tr_{met}
- Calculate Extinction Ratio

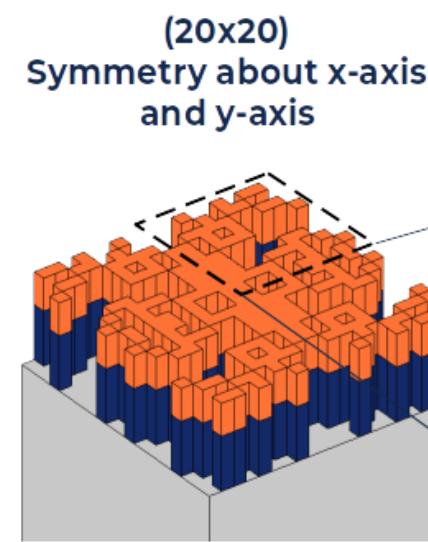


Variable	Value
Insulating $T_{ambient}$	273.15 K (0 deg C)
Metallic $T_{ambient}$	373.15 K (100 deg C)
Time	10 us
Incident power flux	1 kW/cm ²
Wavelength	2.7 μ m
Unit cell dimensions	2 x 2 μ m
Number of sub-pixels	20 x 20
Pixel dimensions	0.1 x 0.1 μ m
Stack-up	Substrate + 400 nm VO ₂ + 240 nm SiO ₂
Number of sims	~15K

Convert Physical Design to Input Image for PerfNN



- Only need one corner of design (symmetry about horizontal and vertical axis)
- Height of layer [nm] at given point is image pixel value
- 2 channels = 2 layers ($\text{VO}_2 + \text{SiO}_2$)



Design as Input Image

(10x10) Channel 0 = 240 nm thick SiO_2

0	240	240	0	...
240	240	240	240	...
0	240	240	240	...
240	240	240	240	...
...

0	400	400	0	...
400	400	400	400	...
0	400	400	400	...
400	400	400	400	...
...

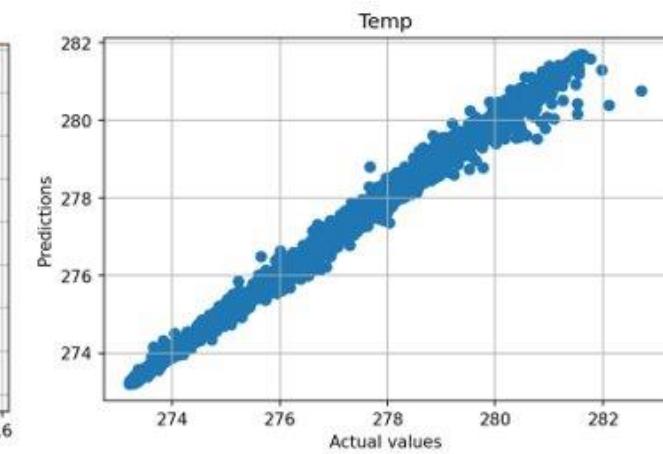
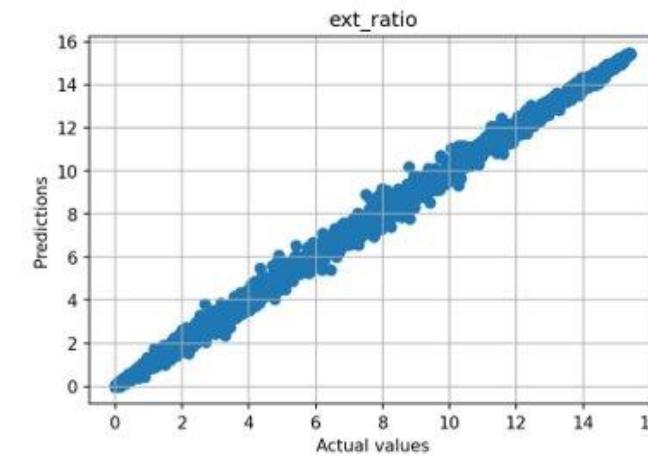
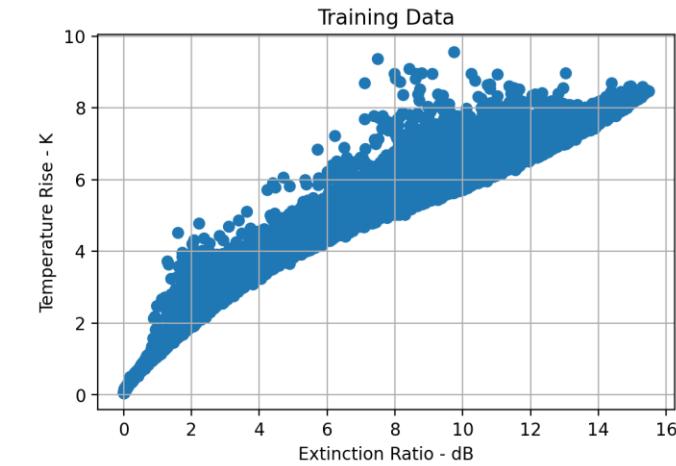
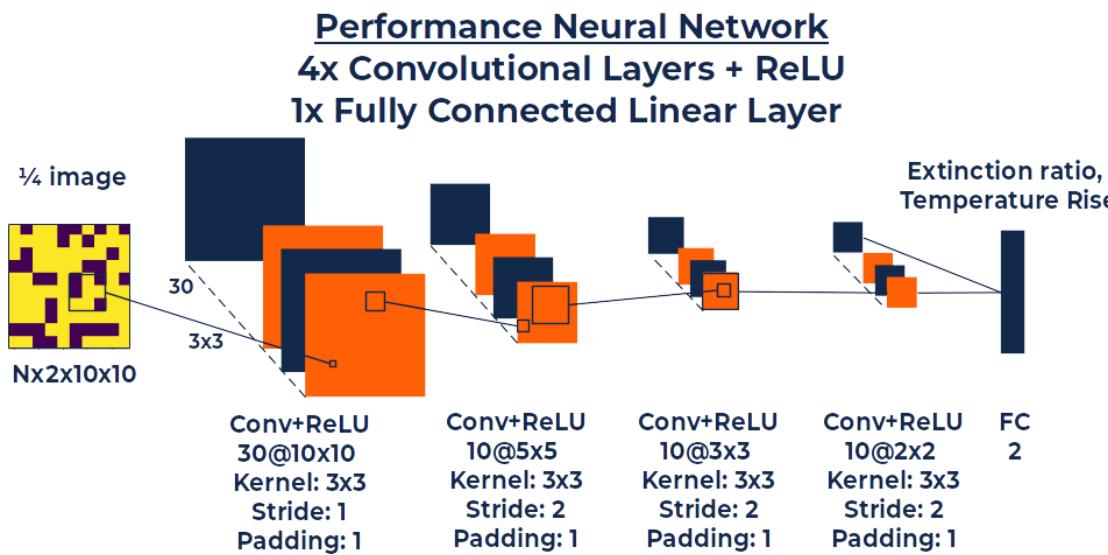
(10x10) Channel 1 = 400 nm thick VO_2

(N,2,10,10)
to PerfNN

Training the Performance Neural Network



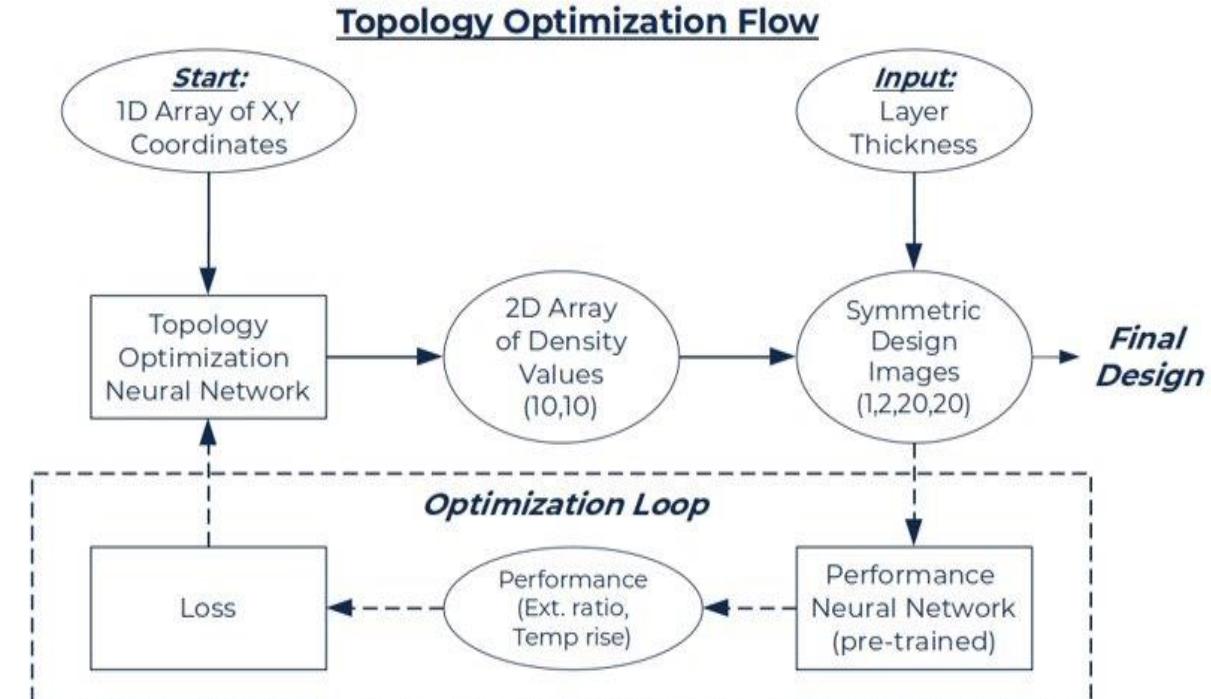
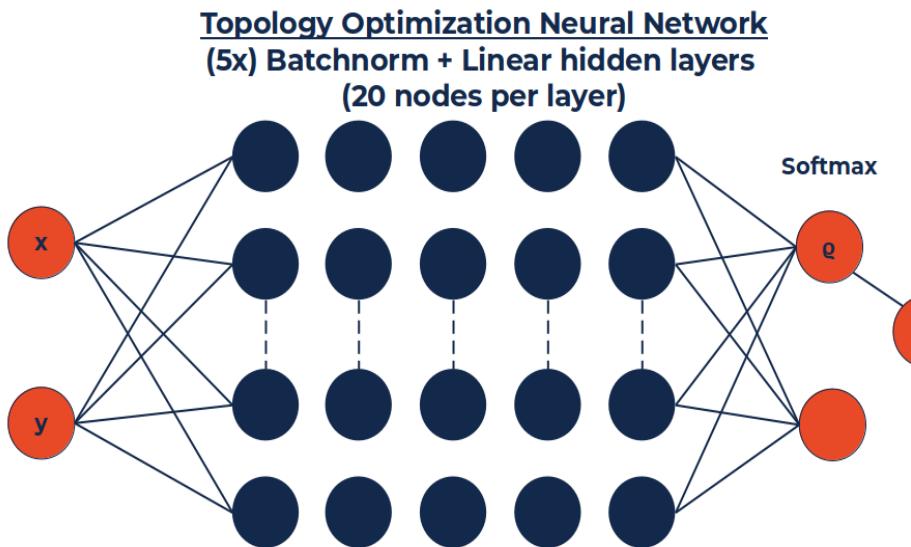
- Train performance neural network
 - Determining what filters to use to best predict performance
 - Backpropagation (automatic differentiation)
- Trained performance
 - Avg abs error: ~13% ext, ~.04% temp
 - Maximum difference: ~1.5 dB ext, ~1.6 K temp



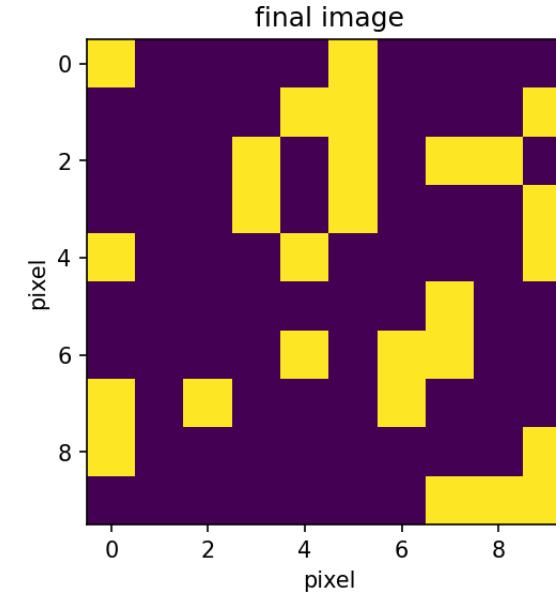
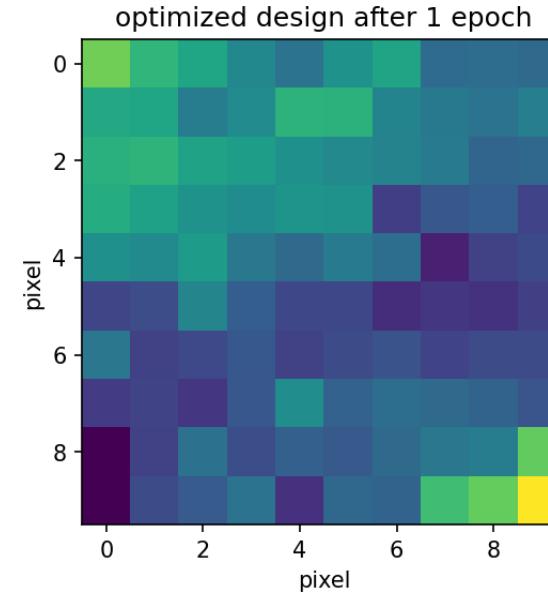
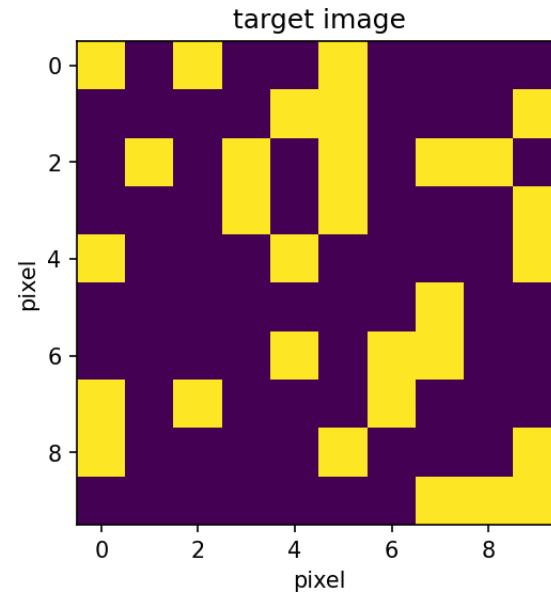
Topology Optimization Neural Network (TopOpt NN)



- Training TopOpt NN
- Each epoch adjusts weights to predict material density at each point

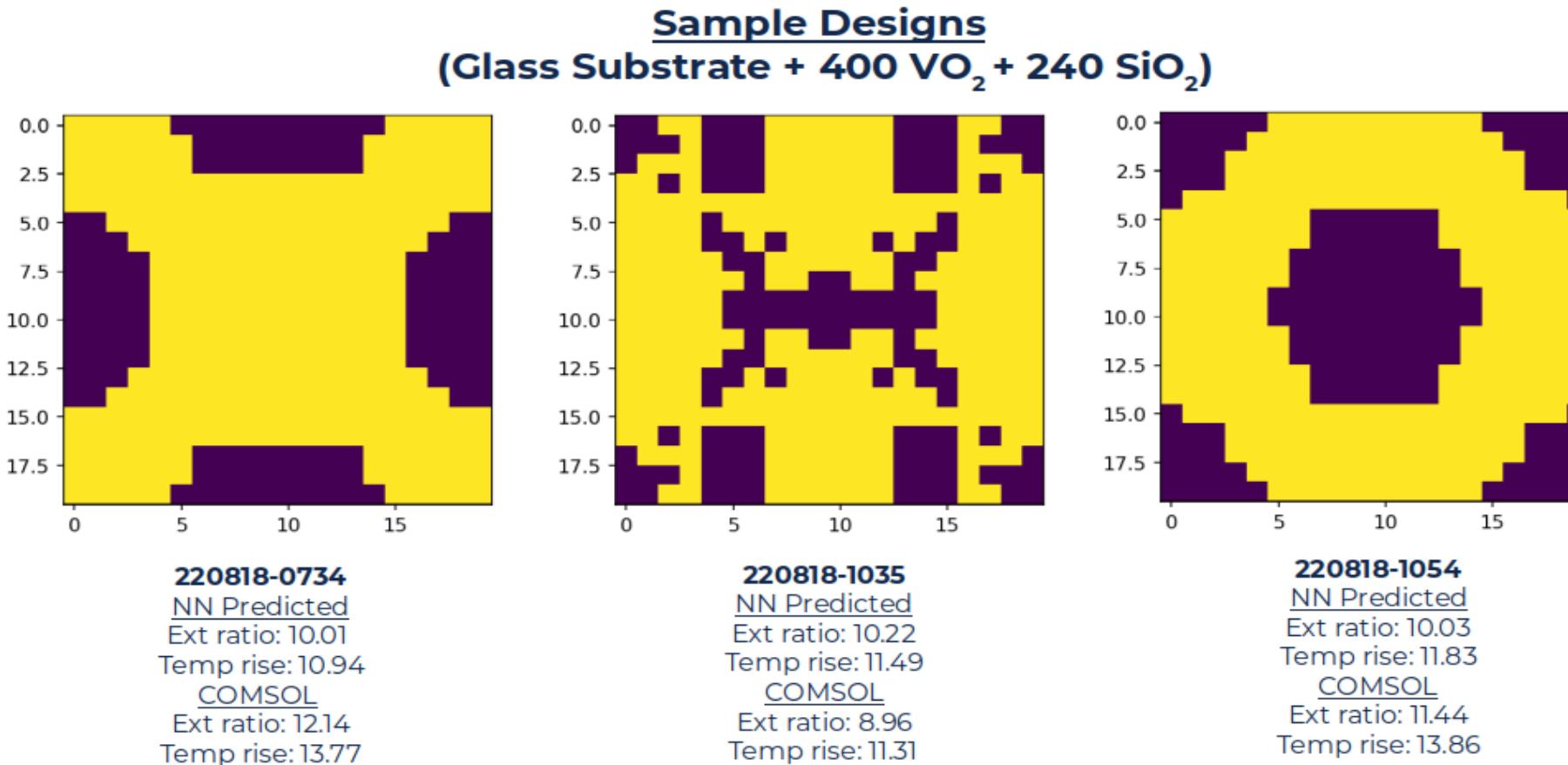


Training the Topology Optimization Neural Network



Test data generated with arbitrary cost function shows good performance

Training the Topology Optimization Neural Network



- TopOpt NN minimizes loss function and provides a proposed (non-unique) solution
- COMSOL confirms that proposed design exceeds performance of training data

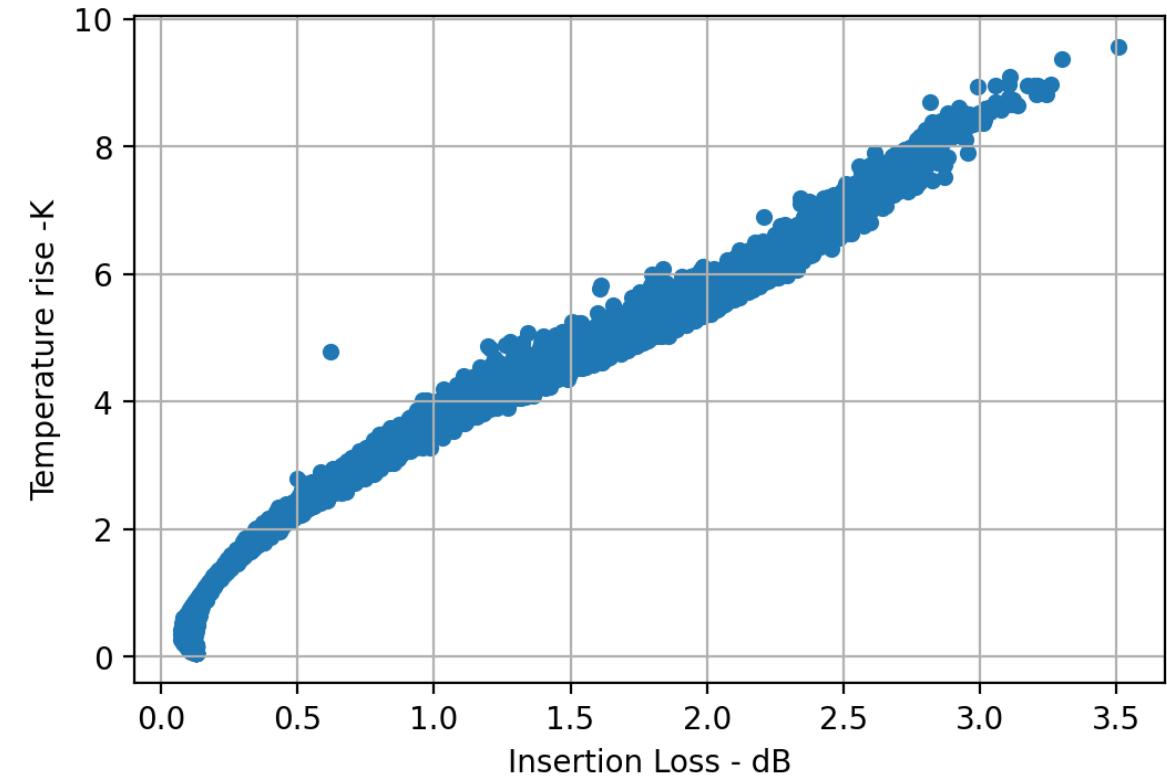
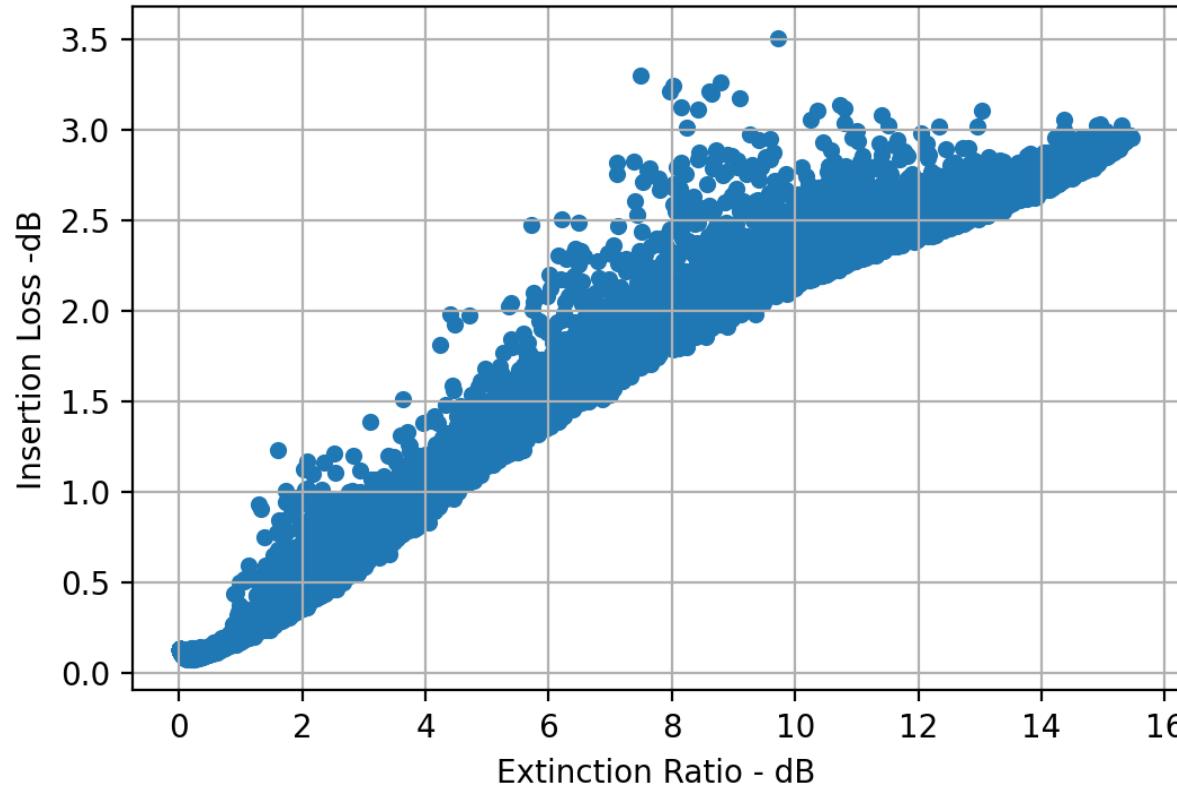
- Fabrication and testing of (3x) designs
- Transfer learning: use simple model to pre-train performance NN and use with more complex coupled EM/thermal time domain simulation
- Expand on use of NN's to solve the inverse design / optimization problem



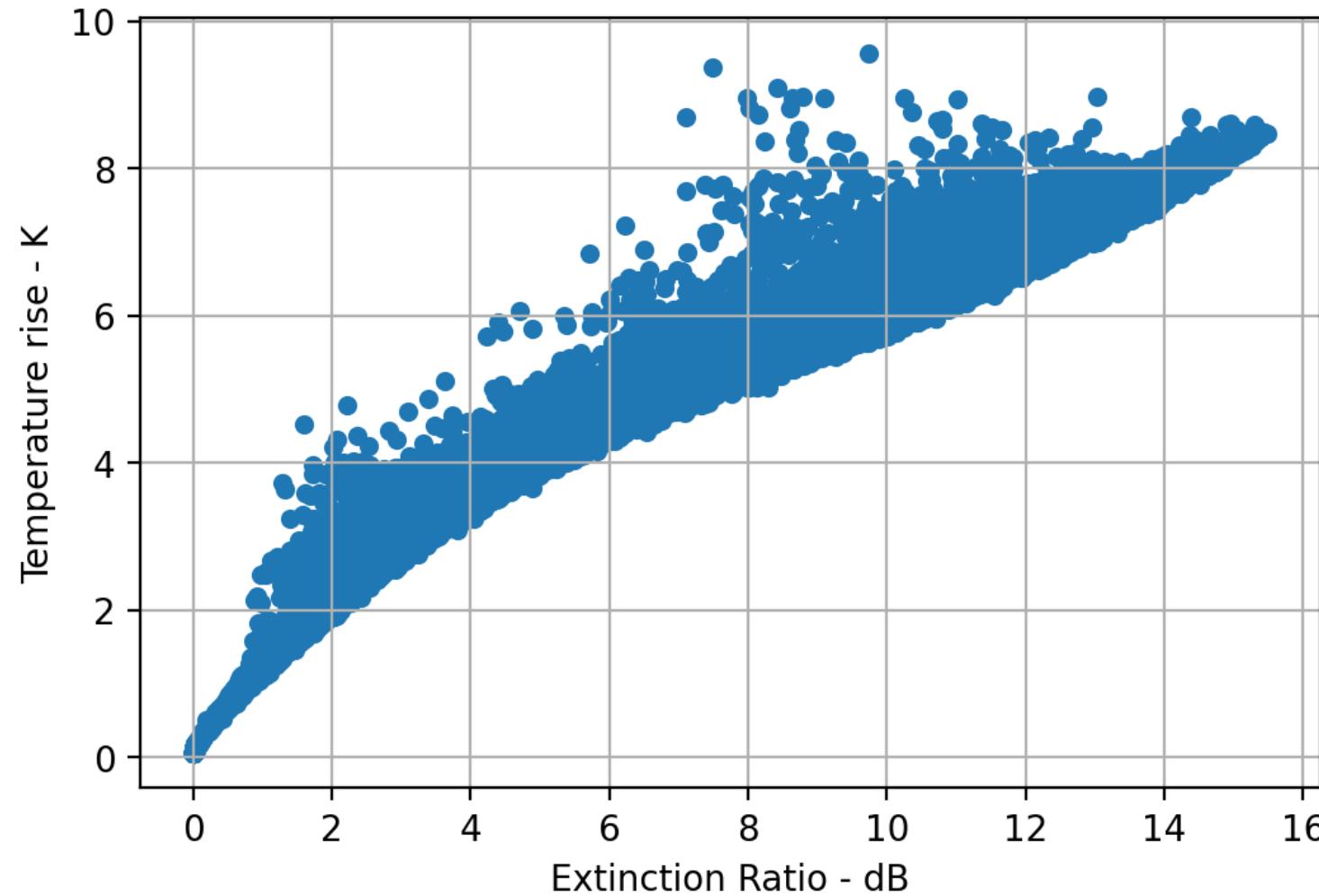
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Training Data



Training Data



Training Data

