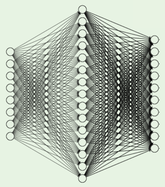

Nanophotonic Particle Simulation andInverse Design Using Artificial Neural Networks

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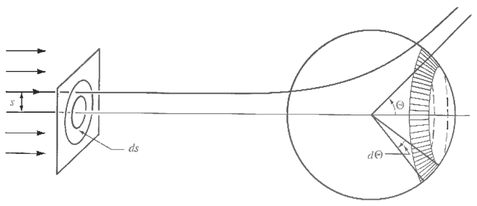
NN's could learn Maxwell's Equations

- Inverse Design is difficult
  - You can compute the forward computation easily in many cases, but going the opposite direction is difficult
- NN's have an analytical gradient/matrix representation, which may be helpful to solve inverse design problems
  - Could Approximation simulations faster
  - Solve Inverse Design more accurately
  - Create an optimizer for desired results.



$$V(\vec{r}) = \frac{ZZ'ee'}{r}$$

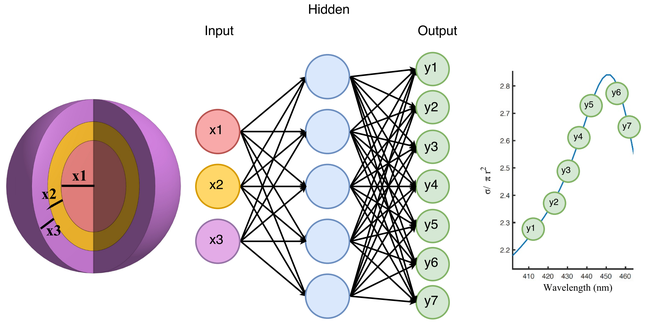
$$\left(-\frac{\hbar^2}{2\mu}\nabla^2 + \frac{ZZ'ee'}{r}\right)\psi(\vec{r}) = E\,\psi(\vec{r})$$

$$\psi(\vec{r}) = e^{ikz}\,g(r-z)$$

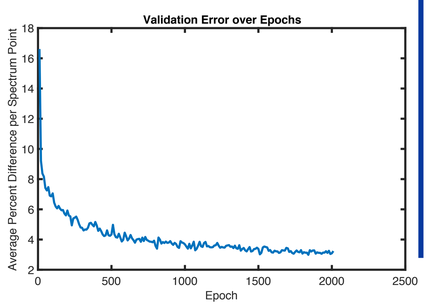
$$\begin{aligned} f(k,\theta) &= -\gamma\frac{\Gamma(1+i\gamma)}{\Gamma(1-i\gamma)}\frac{e^{-i\gamma\log\sin^2\theta/2}}{2k\sin^2\theta/2} \\ &= -\frac{\gamma}{2k\sin^2\theta/2}\,e^{i(\eta_0-\gamma\log\sin^2\theta/2)} \end{aligned}$$

$$\frac{d\sigma}{d\Omega} = \frac{\gamma^2}{4k^2\sin^4\theta/2}$$

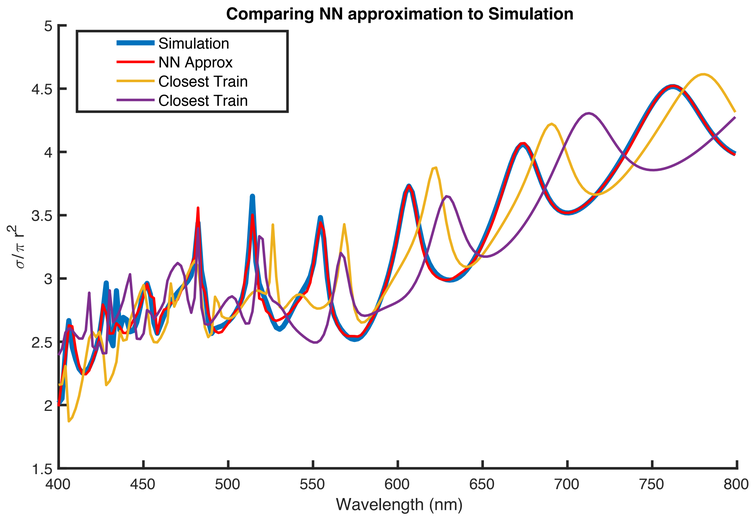
- We show this by solving nanophotonic design.



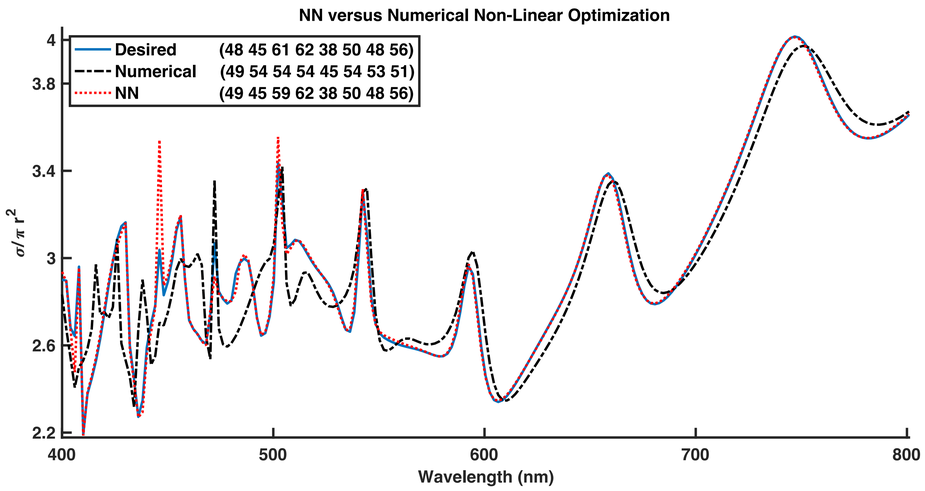
- The geometry (individual layer thicknesses) are input to the NN.
  - 8 layers , 30-70nm thick
  - Alternating TiO2/Silica
- A Matlab simulation generates the training data.
  - ~50,000 examples



NN's solve Nanophotonic Inverse Design



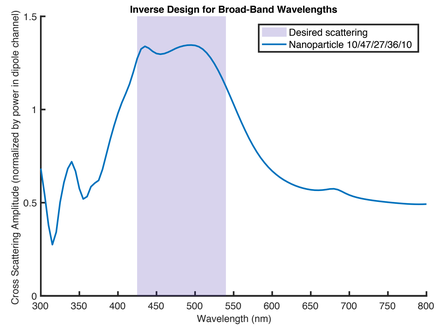
- The yellow/purple line show the nearest training examples in size.
- This had 8 input parameters, and was only shown 50,000 samples (~4 samples/input)



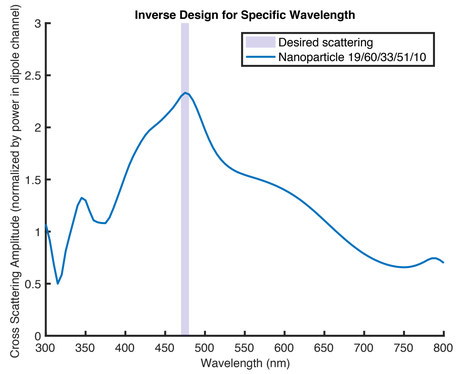
- To solve inverse design, we fix the weights and train the inputs as biases
- This result is for an eight layer nanoparticle.
- Blue is the desired spectrum, the black is from numerical non-linear optimizations, and the red is the Neural Network results.
  - This was compared against interior-point methods, initialized 50 times

NN's can be an Optimization Tool

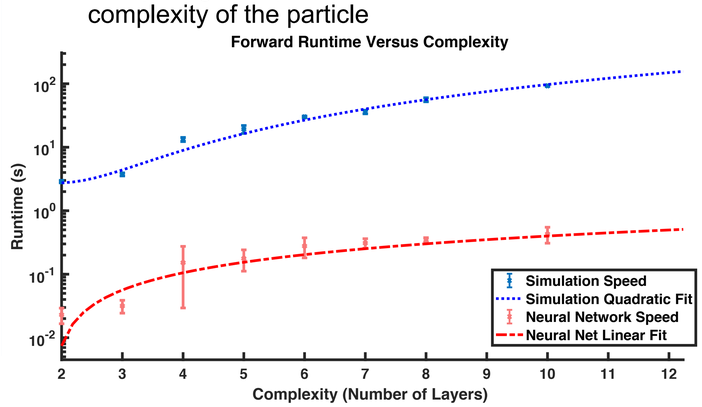
- We choose a loss function to optimize for a particular scattering



- The cost function here was maximizing purple region, minimizing outside.
- After a couple of iterations, it finds a broad-band material.
- Similarly, the procedure can be used for specific-wavelength scattering
- Applicable even if the underlying materials do not have sharp resonances

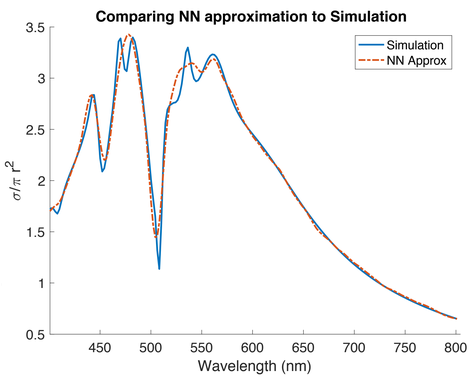


- Comparing the speed of the simulation/NN versus complexity of the particle



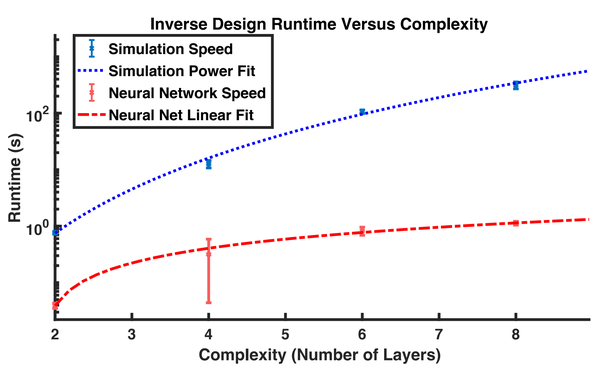
Exotic Materials: J-Aggregates

- Nanoparticles made with J-Aggregates have sharp resonances.
- Sharper resonances made the spectrums vary greatly
- NN still well-behaved.
  - Trained on same number of examples.
  - Only 3 layer particle
    - Metal, Dielectric, J-Agg



Inverse-Design Speeds

- Comparing time to reach a desired threshold



Conclusions

- Demonstrated NN can learn/approximate Maxwell interactions
- Showed NN's can solve Nanophotonic Inverse Design
- Constructed broad-band and specific-wavelength materials.
- Compared the speeds, and suggested that NN can open up previously insolveable inverse design problems.

Acknowledgements

This material is based upon work supported in part by the National Science Foundation under Grant No. CCF-1640012, as well as in part supported by the Semiconductor Research Corporation under Grant No. 2016-EP-2693-B. It is also supported in part by the U. S. Army Research Laboratory and the U. S. Army Research Office through the Institute for Soldier Nanotechnologies, under contract number W911NF-13-D-0001, as well as in part by the MRSEC Program of the National Science Foundation under award number DMR - 1419807.

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NIPS Dec 7th, 2017