Connecting numerical simulation and machine learning: How to bridge the gap between theory and reality?

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Abstract – **Machine learning and numerical simulation represent opposite approaches to computational analysis of the real world, inductive vs. deductive. However, both methods suffer from various uncertainties and even their combination often fails to link theory and reality. This paper presents a critical review of such connections and proposes improvement options for optoelectronic devices.**

Index Terms **— machine learning, deep learning, neural networks, artificial intelligence, numerical simulation, semiconductor, optoelectronic devices, photonics**

Numerical simulations embed theoretical models into a practical environment. This enables a realistic test of such models by comparing calculated results to measurements. Simulations can thereby help explain experimental results that would otherwise be hard to understand. Simulations also allow for performance predictions of novel devices. However, it is well known that initial simulations hardly ever agree with experimental results. Possible reasons for such disagreement are manifold: incomplete or incorrect models, unrealistic parameters, and/or computational mistakes. Besides measurement errors, reasons on the experimental side include insufficient knowledge of the actual device structure and/or of the experimental procedure. Anyway, numerical simulations often fail to represent the real world and create a virtual reality instead (Fig. 1).

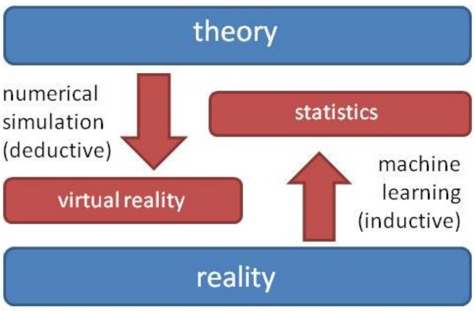

Fig. 1: Deductive vs. inductive method.

Machine learning, on the other hand, usually collects data in the real world and performs statistical analyses (Fig. 1). This is especially valuable when the amount of data is very large and hard to digest. Deep learning is currently the most popular machine learning method and it is based on multi-layered artificial neural networks (ANNs).[1] But this black-box approach ignores any existing theoretical model. ANNs simply transfer input numbers into output numbers without regard for their meaning. Thousands of data sets are required to train an ANN. However, final predictions are often unreliable.[2]

In order to alleviate some of these uncertainties, data collection from the real world is often replaced by numerical simulation, thereby producing theoretically consistent data sets for ANN training. Various publications in materials science demonstrate this approach.[3] Real-world data shortage and data scattering are circumvented this way, but at the expense of realism.[4] Machine learning from flawed simulation models renders such flaws invisible and untraceable.[5]

The situation is similar with photonic devices, as experimental ANN training is hardly performed.[6] Simulation-trained ANNs are often employed to speed up design optimizations. Examples have been published in fiber-optics,[7] integrated photonics,[8] nano-photonics,[9] plasmonics,[10] and meta-materials.[11] Some authors embed ANNs in their numerical procedure to reduce the parameter space.[12] All these applications in photonics are based on solutions to Maxwell's equations that involve only few material parameters, namely refractive index and absorption coefficient. However, these parameters depend not only on the material, but also on the optical wavelength, on the ambient temperature, and possibly on the optical intensity and on processing. Variations often require a time-consuming ANN retraining. While gaining speed in the final design optimization, modeling flexibility is lost as well as theoretical insight. Plus, scientific discoveries are unlikely because ANNs typically interpolate between known numerical results.

Compared to photonic devices, optoelectronic devices are much more complex as they combine optical, electronic, and thermal processes. Their self-consistent simulation not only involves various modeling approximations in need of validation, but also a large number of uncertain material parameters. Therefore, design optimization strategies known from photonics[13] are hardly applied in optoelectronics.[14] However, simulation-based machine learning methods have been utilized in the design of laser diodes,[15]

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semiconductor optical amplifiers,[16] light-emitting diodes,[17] and solar cells.[18] In case of the laser example, the authors try to deduce the laser design from the desired light-current (LI) characteristic. But instead of typical design parameters such as wavelength, materials, layer thicknesses, and facet reflectivity, practically unknown modeling parameters are used for ANN training, such as injection efficiency and temperature coefficients.[15] Based on such training, the inverse ANN design produces many broadly scattered parameter sets for the same LI characteristic. Further machine learning pitfalls in optoelectronic device design are evaluated elsewhere.[19]

Most of these examples operate within the virtual reality created by numerical simulations (Fig. 1). The quantitative validation of models and results by measurements is missing. In order to achieve more realistic predictions, several improvement options are suggested in the following.

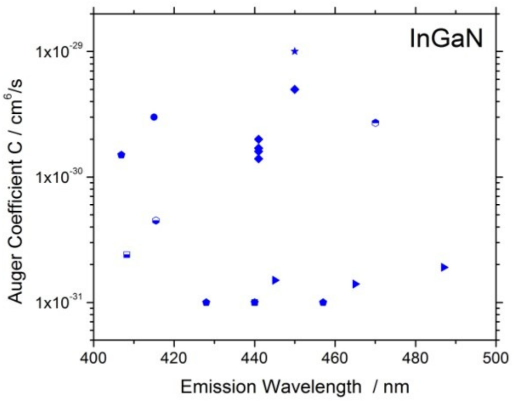

Fig. 2: Reported Auger recombination coefficients.

A main source of simulation uncertainties are the material properties used in the model. Published values of some key parameters scatter widely (Fig. 2).[20] The analysis of such variations as well as their implementation in the numerical procedure can help establishing error ranges for simulation results.[21]

The Materials Genome Initiative provides many good examples for the synergetic combination of theoretical models, computational methods, and experimental procedures.[22,23] This may lead to more reliable models of optoelectronic material properties employable by device simulations.

Key processes in optoelectronic devices, such as the optical gain, are often represented by simplified models to reduce the computation time of full device simulations. High-end models for such complex processes can be calculated separately and then imported into the device simulation via ANN or other suitable means.[24]

Assumptions about the simulated device are usually based on design intentions and not on the structure actually fabricated, hindering a comparison between simulation and experiment. Typical examples are layer thicknesses, material compositions, and doping profiles. Direct measurements of such structural data should be preferred in the simulation setup, whenever possible.

The initial disagreement between simulation results and performance measurements is often eliminated by adjusting parameters in the model.[25] However, this is a slow iterative process mostly based on intuition. Each parameter usually requires a different measurement for calibration. Such multi-dimensional fitting procedure opens the door for machine learning from experimental data. As most material parameters change with temperature, improved strategies are especially needed when thermal effects are relevant.

The industrial fabrication of optoelectronic devices often includes the automatic acquisition of performance data from various measurements. Some data scatter significantly, which may be related to unintended processing fluctuations. ANNs can be used to analyze such experimental variations and, e.g., select the set of measured data that is most appropriate for evaluating and calibrating simulations.

Generative adversarial networks (GANs) are increasingly popular in deep learning applications.[26] They may be able to combine simulation-based and experimental input and help linking theory and reality.

In conclusion, the popular combination of inductive and deductive computational methods typically suffers from an insufficient inclusion of experimental data. Several approaches are proposed to bridge the resulting gap between theory and reality, which is expected to improve the impact and the reputation of numerical simulations.

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