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# Machine-assisted design and stochastic analysis in integrated photonics

(Invited paper)

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## ABSTRACT

Integrated photonic devices are steadily making their way into many application fields including modern optical communication networks and advanced sensors. On the other hand, the design of photonic devices and circuits mostly remains a time-consuming process largely based on the designer experience. This limits the size and complexity of the parameter space that can be handled. Moreover, addressing the effect of manufacturing variability remains a fundamental challenge since small fabrication errors can have a significant impact on light propagation, especially in high-index-contrast platforms such as silicon-on-insulator. The analysis of this variability with conventional approaches (e.g. Monte Carlo) can become prohibitive due to the large number of required simulations. Recent advances in machine-assisted design methods are opening the possibility to vastly expand the number of design parameters, exploring novel functionalities and non-intuitive geometries. In this invited talk we discuss the use of machine learning methods for the design of integrated photonic devices. We show the existence of a large number of possible designs that are all equivalent with respect to a given primary design objective but with distinct properties in other performance criteria. We use pattern recognition to reveal their relationship and to reduce the dimensionality of the large design space by properly defining new design variables. Likewise, we show how efficient stochastic techniques allow a quick assessment of the performance robustness and the expected fabrication yield for each tentative device. We focus in particular on stochastic spectral methods that have been regarded as a promising alternative to the classical Monte Carlo method, achieving a considerable reduction of the simulation time. Together, the reduction in the design space dimensionality and efficient stochastic techniques allow for the integration of the fabrication tolerance considerations into the design process.

**Keywords:** photonic devices, silicon photonics, machine learning, stochastic processes, pattern recognition, uncertainty analysis.

## 1. INTRODUCTION

The design of novel photonic devices with complex and non-trivial geometries vastly increases the number of design parameters and makes manual device design impractical. Tools such as the genetic algorithm, particle swarm, gradient-based optimization, and artificial neural network are often used to search more efficiently for high-performance designs [1]. Highly compact devices employing non-intuitive geometries have been demonstrated exploiting inverse design methods. [2]. However, the ability to efficiently explore and comprehend large design spaces is still beyond reach. Moreover, the analysis of the impact of manufacturing variability remains a major challenge [3]. Classical methods for stochastic analysis such as Monte Carlo require a very large number of simulations to obtain reliable results, hampering their use in large-scale multi-parameter designs.

In this invited talk we report on the application of advanced computational approaches for the design and analysis of photonic integrated devices. We show that applications of machine learning tools can benefit the design of devices with a large number of parameters. We investigate the study case of a vertical grating coupler made in silicon-on-insulator technology [4] using a suite of machine learning tools, including global optimization, supervised learning and unsupervised machine learning pattern recognition. Starting from a small set of possible alternative designs with state-of-the-art fibre coupling efficiency we analyse the apparent

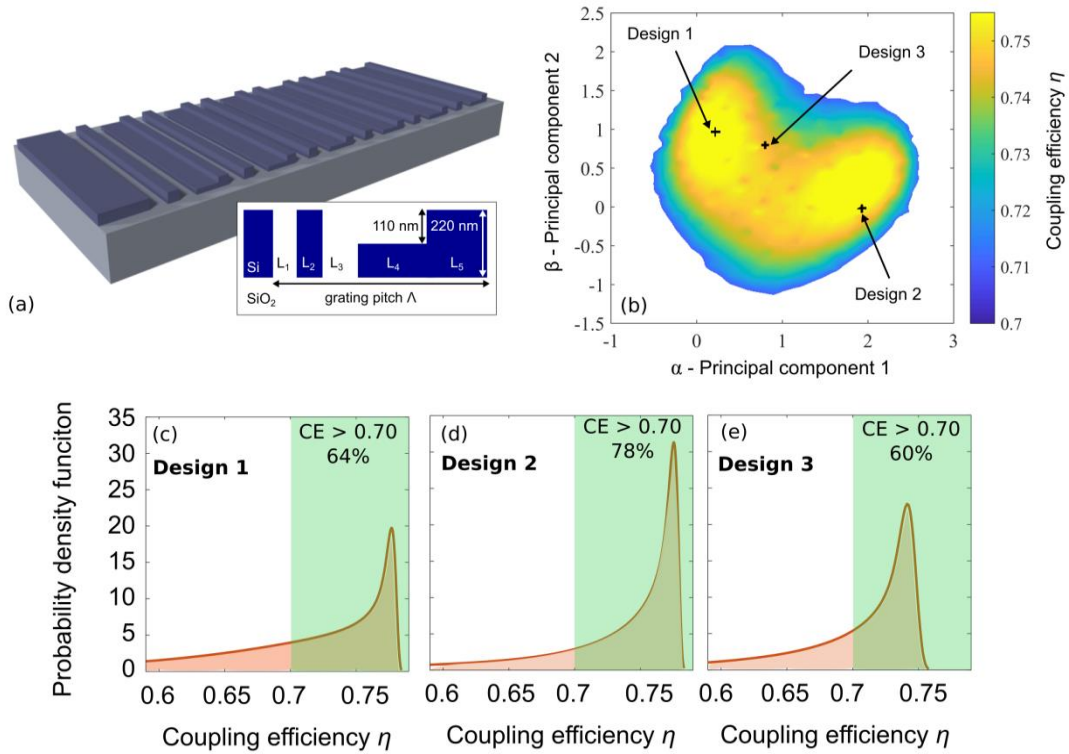


Figure 1. (a) Schematic of the vertical grating coupler. The design involves five parameters (the length of each section  $L_1$ - $L_5$ ). (b) Using a combination of machine learning techniques, including pattern recognition, the 5-D design space can be efficiently explored, identifying a 2-D sub-space (hyperplane) containing a large number of alternative grating designs all with a state-of-the-art fibre coupling efficiency larger than 0.7. (c)-(e) Probability density function of the coupling efficiency for the three designs highlighted in (b) when a standard deviation of 5 nm for the segment lengths is considered. The three designs have different fabrication yield, calculated as the probability for the device to have a coupling efficiency larger than 0.7 for the three designs (green shaded areas).

redundancy of the original five-parameter design. This analysis reveals that all good designs belong to a 2D hyperplane, a subspace within the 5D design space. Such reduction in dimensionality allows us to perform exhaustive evaluation of the subspace of good designs and identify design candidates with equivalent fibre efficiency but significant differences in other criteria such as back-reflection or robustness to fabrication variability [4].

Starting from these results, we then present the application of polynomial chaos expansion (PCE) techniques to investigate how the device performance deteriorates in the presence of dimensional variability due to fabrication uncertainty. PCE allows building a surrogate model of an unknown random function by representing its dependence on stochastic variables using an orthogonal set of polynomials. With a very limited number of initial simulations PCE provides an accurate representation of the variability, predicting its effects on the final designs and enabling the computation of stochastic quantities such as fabrication yield.

## 2. STOCHASTIC ANALYSIS IN HIGH-DIMENSIONAL DEVICE DESIGN

Figure 1(a) shows the vertically-emitting grating coupler considered here as a study case. The grating period consists of a pillar of 220 nm in height and an L-shaped section partially etched to 110 nm whose blazing effect ensures that light is primarily diffracted upwards. The structure dimensions  $L_1$  -  $L_5$  define the five-dimensional design parameter space. The design objective is the coupling efficiency CE of the diffracted TE-polarized light to a standard single mode optical fibre (SMF-28) placed vertically on top of the grating. As described in [4], a machine-learning enhanced search allows finding a collection of different good designs whose coupling efficiency is between 74% and 76%. Although coupling efficiency is the primary performance criterion for these kind of devices, there are several other important considerations to take into account, whether application specific (e.g. very low back reflections, high bandwidth) or mandated by the manufacturing process (e.g. feature size limitations). Obtaining a characterization of the subspace of good designs can significantly clarify the situation as trade-offs between various considerations become easier to calculate and visualize. For this purpose, we apply the dimensionality reduction technique within the unsupervised machine learning toolbox, specifically the principal component analysis (PCA) [5]. PCA finds a sequence of best linear approximations to the dataset

based on minimizing the least squared errors and the results explicitly show how many orthogonal linear projections are needed to represent the dataset within a certain level of accuracy. For the collection of good grating designs described above, 5 different designs are enough for PCA to reliably reveal a two-dimensional subspace that contains all possible designs with state-of-the-art coupling efficiency, and thereby excludes a large part of the design space that is no longer relevant. A reduction from five dimensions to two allows us to perform an exhaustive performance evaluation of all the designs included in the lower-dimensional subspace and generate for coupling efficiency the map shown in Fig. 1(b) using less than 1000 simulation runs. Alternatively, a similar exhaustive scan in five dimensions would require millions of simulation runs to identify the region of good designs with the same level of accuracy. The exhaustive scan of the 2D subspace identified by the PCA provides a complete map of the subspace of good designs and naturally makes it easy to choose the design to fabricate given a complete set of requirements and constraints. For example, designs 1 to 3 highlighted in Fig. 1(b) have very similar coupling efficiency of 76%, 75.5% and 74.5%, respectively, but very different back-reflections (-21dB, -40dB, and -17dB). Also the tolerance to fabrication variability is different between the three designs, as described below. Some interesting insights about a range of possible good designs can be obtained even before the exhaustive scan is performed. For example, it is straightforward to identify various minimum feature sizes that good devices can possibly have by inspecting the 2D subspace without the need to run any optical simulation. In particular, this specific grating architecture does not have good designs with a minimum feature size larger than 90 nm.

While coupling efficiency has been treated so far as a deterministic quantity, it is unavoidably subject to variability due to dimensional variations during fabrication. We can efficiently investigate this variability by computing a surrogate model for coupling efficiency exploiting a polynomial chaos expansion technique [3]. We consider coupling efficiency CE at  $\lambda = 1550$ . We assume for both shallow and deeply etched sections in the grating the same random width deviation  $\delta$ , normally distributed with zero mean and a standard deviation of 5 nm. For the coupling efficiency, a polynomial order  $P = 3$  (4 coefficients) is enough to provide a good fit. To robustly estimate the four coefficients by means of linear regression 8 values for  $\delta$  are sampled according to its distribution and the corresponding designs are simulated with 2D-FDTD. The computational time required to build the surrogate model is negligible compared to optical simulation time. The entire analysis is performed with a number of simulations orders of magnitude smaller than Monte Carlo, making its application to the large number of designs shown in Fig. 1(b) possible with only a few thousands of optical simulations. Figure 1 (c)-(e) shows the probability density functions of coupling efficiency for designs 1, 2, and 3 highlighted in Fig. 1(a). The probability density functions are obtained by sampling the surrogate models 5000 times (which only takes a few seconds) and using a Gaussian kernel density estimator. During the analysis, fabrication yield is also estimated for the criterion of  $CE > 0.7$ . The number of devices respecting this criterion (yield) is computed integrating the corresponding part of the probability density function. Design 1 shows a longer tail towards lower values of CE compared to design 2, reducing the probability to obtain a high coupling efficiency and consequently the yield (64% instead of 78%). Design 3 has the lowest average coupling efficiency (68%) and the lowest yield (60 %).

### 3. CONCLUSIONS

We have shown how the introduction of machine learning tools in the design of photonic devices brings unparalleled capabilities in terms of speedup in the exploration of large design spaces and physical insight of non-intuitive geometries. Likewise, polynomial chaos expansion can be fruitfully exploited to efficiently investigate the stochastic properties of photonic devices and circuits subject to fabrication uncertainty. This makes the approach attractive for the investigation of large multi-parameter design space and machine-assisted design approaches requiring the analysis of a large number of possible alternative design solutions.

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