PRINCIPAL COMPONENT ANALYSIS AS A POST-PROCESSING TOOL IN MICRO- AND NANO-PHOTONICS MEASUREMENTS AND MODELIZATIONS.

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The signals typically extracted from nano-devices are weak and can be strongly masked by noise, presenting a low signal-to-noise ratio. Computational electromagnetism and high resolution measuring techniques in Nano-Science an Nano-Technology produce a large amount of data that needs dedicated post-processing to enhance pure spatial, pure temporal, or mixed spatial-temporal structures embedded in the data. The Principal Component Analysis (PCA) has been proved in other fields as a very useful tool able to reveal inner correlations, and hidden structures in very large data sets. Among other applications, PCA has been used to characterize spatial-temporal patterns of noise in visible and infrared imaging devices.¹⁻³ In this contribution, we offer an statistical technique, the PCA, that is well suited to extract useful information, even from faint signal embedded in noise but having a non negligible degree of correlation. PCA is blind in nature, i.e., it does not need any prior preparation of the analyzed data. However, the correct interpretation of the results requires some knowledge of the physics and technology supporting the studied phenomena. We show how PCA is useful for a variety of Nano-Science and Nano-Technology applications. The cases treated here involve a large amount of numeric data, and experimental techniques dealing with weak signals and strong noise structures.

Firstly, we have applied the PCA to the output of computational electromagnetism algorithms. This application is quite similar to the one already tested in the analysis of sequences of frames generated by imaging acquisition devices. The presence of noise and artifacts generated by the numeric discretization and implementation of Finite-Differences Time-Domain methods⁴ has been quantified and spatially localized with subwavelength accuracy.⁵ Moreover, the application of PCA to the electromagnetic field computations, has revealed the existence of stable electromagnetic field distributions different from the mode defects already appearing in the structure.⁶ These spatial-temporal patterns have been also related with the spurious presence of modes different than those excited within the bandgap. The fine resolution of the method is able to enhance structures with a very low contribution (lower than 10^{-4}) to the total variance of original data but having strong correlation. This is the case of the appearance of whispering gallery modes in the central defect of a photonic crystal (see figure 1).

Besides of this numeric application, we have applied the PCA method to the extraction of relevant features in the measurement of micro-structures with nano-resolution techniques, as the atomic force microscope mapping. We will present the results obtained for the dimensional characterization of a metallic wire with an atomic force microscope. At the same

time we will show how the PCA method has been crucial to define a safe and sound method in the measurement and characterization of micro- and nano-infrared-antennas.⁷ This example is interesting from a metrologic point of view. It establishes how the experimental and equipment uncertainties can be included along the process, from the data acquisition to the final parametric characterization of the results. Even when a highly non-linear module, as an iterative deconvolution process, is included in the characterization chain.

References:

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Figure 1: Left: plot of the Poynting vector inside the cylinders of a photonic crystal microcavity. Right: Electric field distribution inside a cylinder of the same photonic crystal showing a whispering gallery mode distribution. These field distributions represent less than 10^{-4} of the total variance of the original sequence of FDTD simulations. However, due to their non-negligible correlation along the data set, they are revealed by the PCA method.