Machine Learning-based Diffractive Imaging with Subwavelength Resolution

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Abstract: We report detection and characterization of wavelength-scale objects with subwavelength resolution by combining diffractive imaging and machine learning. The technique clarifies the information channels in the diffraction imaging and provides insight into machine learning processes.

Optical microscopy provides unparalleled tools for understanding and characterization of small-scale objects [1-3]. The resolution of conventional (refractive) microscopy is typically limited to \( \approx \frac{\lambda_0}{2NA} \) with \( \lambda_0 \) being the free-wavelength and \( NA \) – the numerical aperture of the objective [1]. Numerous techniques, primarily based on multiple measurements of the same object, to achieve subwavelength resolution, have been reported [2]. Theoretically, the ultimate far-field resolution limit has been related to the signal-to-noise ratio of the measurement technique [3]. Interscale mixing microscopy (IMM)[4,5], a technique based on the analysis of the object’s interaction with a finite-size diffraction grating, has been demonstrated as a powerful tool for characterizing one-dimensional objects with a resolution of approximately \( \lambda_0/10 \) with a single measurement. However, straightforward mapping of IMM to two-dimensional objects is practically impossible. Here we demonstrate, both theoretically and experimentally, that IMM-inspired diffractive imaging can be extended to two dimensional objects by employing machine-learning techniques. The proposed approach not only provides a practical solution for the important problem but also yields an important insight into the information flow in diffraction microscopy and into the machine learning process itself.

The diffractive imaging setup, along with the typical samples used in our studies, are illustrated in Fig.1. Individual samples represent 11x11 arrays of apertures (period \(~300\text{nm}\), diameter \(~150\text{nm}\)) fabricated using focused ion-beam milling, similar to that used for 1D structures [4]. Some of the apertures in the samples are blocked, representing the subwavelength objects to be characterized by the system. Overall, 14 structures representing 12 different arrangements of the defects were fabricated and characterized.

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Figure 1: Panel (a) illustrates experimental setup (main figure) and several examples of the diffractive structures analyzed in our experiments (right insets); typical processed diffractive intensity patterns are shown in panels (b) (theory) and (c) (experiment); panels (d,e) illustrate the main result of this work, the average contribution of the information contained in a given \( m,j \) pair to the recovery accuracy, as indicated by analysis of theoretical (d) and experimental (e) data; both panels (d,e) represent averages of multiple recovery attempts with different combinations of Bessel harmonics. Inset in (e) illustrates one such individual study as described in the text.
The samples are characterized by the diffractive imaging Fourier spectroscopy setup, as shown in Fig.1a with laser light with $\lambda_0 = 532nm$, making the diameter of the individual defect $\sim \lambda_0/3.5$. Fig.1c shows a typical diffraction pattern recorded by the CCD. Attempts to generalize the analytical approach introduced for one dimensional objects in Ref.[4] have been unsuccessful since the generalization of the analytical IMM formalism calls for multiplication by $\sin k_x A \sin k_y A$ thus eliminating all major maxima in the diffraction pattern, and significantly reducing the usable signal. Therefore, instead of generalizing the analytical formulation of IMM to 2D systems, we utilize a machine learning paradigm to recognize diffractive signatures of sub-wavelength objects.

Idealized diffraction patterns of the samples used in the study have been generated theoretically (Fig.1b). To mimic the finite resolution of the ion-beam milling several (10…100) theoretical diffraction patterns were generated for each experimental configuration. In these ensembles, the position of the apertures were varied by 2.5nm along each lateral direction, while the radii of the holes were varied by 10nm. Parameters of the Discrete Fourier Transform were chosen to match the finite resolution of the CCD used in our experimental setup.

To further classify the images and to analyze the information flow in diffraction imaging, the intensity recorded by the CCD has been post-processed to enhance the diffracted signatures, and the resulting patterns have been represented as a linear combination of Bessel functions:

$$\tilde{I}(k_x, k_y) \approx \sum_{m,j} C_{m,j} J_m(\frac{kr}{k_0}) \cos(mx)$$

with $(k_x, k_y)$ representing the position of the processed intensity within the CCD, indices $m, j$ describing the angular and radial behavior of the intensity, respectively, parameter $k_0$ describing the lateral size of the pattern, and $\alpha_{m,j}$ being $j$-th zero of Bessel $J_m(x)$. Note that the coefficients $C_{m,j}$ are independent of each other and are calculated using standard Fourier-Bessel transform techniques.

Characterization of the small-scale objects embedded into diffraction grating can now be formally mapped to the supervised machine learning (ML) paradigm. In this approach, the ML algorithm is first trained on the signatures of the properly selected set of $C_{m,j}$ coefficients representing theoretical patterns of known samples. Then the trained classifier is utilized to characterize either the subset of theoretical patterns or the experimental patterns based on their signatures representing the same set of $C_{m,j}$ coefficients. Importantly, by analyzing the performance of such classifier we can identify the set of Bessel harmonics responsible for carrying the information about identifying features of the source.

The data summarizing multiple runs of the Support Vector Machine (SVM) classifier with different combinations of the $m,j$ pairs are summarized in Fig.1(d,e). Each point $(M, f)$ in the inset of Fig.1e represents the classification accuracy when training and recovery are performed based on 100 components of Bessel expansions, with $m = M \ldots M + 10, j = J \ldots J + 10$. The panels (d,e) represent averages over multiple training/recovery attempts with different combinations of Bessel components, and thus represent the contribution of each component into the overall recovery efficiency. Note that the parameters optimizing the performance of theoretical models also optimize the classification of experimental sets despite significant noise and glare-type artifacts present in the experiment (Fig.1c).

Under close to optimal conditions, the developed algorithm is capable of accurately characterizing 12 out of 14 samples, including the samples with single closed aperture, based a single diffractive pattern per sample. This optimal recovery rate far exceeds the values reported for subwavelength imaging of isolated objects [3] and illustrates the strong enhancement of subwavelength information in the far-field signatures, promoted by the finite-size gratings. Finally, we note that the robustness of linear SVM as compared to its Gaussian counterparts indicate that the Bessel-based parameterization of the diffractive imaging is close to optimal representation of the structural information.

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