## Physical inference from multidimensional photoemission data

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Multidimensional photoemission spectroscopy (MPES) is a unique and powerful technique in condensed matter physics for the comprehensive momentum space mapping of electronic band structures in three or more dimensions [1]. The experimental photoemission spectra capture the singleparticle and many-body electronic signatures of materials in and out of equilibrium [2]. The increasing scale and complexity of the photoemission data produced by the latest generation of instruments present fresh challenges to the existing analytical methods in the photoemission community developed over the past decades, which focus mostly on individual and localized spectral features [3]. A global understanding and exploration of the multidimensional photoemission data requires new approaches. On the other hand, machine learning and computer vision algorithms that power the facial recognition systems and self-driving cars are emerging as precision methods to seek and answer complex scientific questions hidden in the experimental data. However, so far, their contributions to the understanding of experimental physics mostly concern the fields of astrophysics, particle physics and quantum computing [4]. In this project, we use photoemission data as information-rich examples in condensed matter spectroscopy to design and tune efficient algorithms that combine machine learning and computer vision with physical prior knowledge to quantify changes and infer physical models and parameters [5]. In doing so, we hope to drive closer the comparison between theory and experiment and to motivate their further developments. At the same time, the scenarios encountered in this arena, such as limited ground truth and imperfect theory for validation, can also stimulate the developments in machine learning to better serve the needs of materials science, other physical sciences and beyond.



References: [1] G. Schönhense et al. J. Electron Spectrosc. Related Phenom. 200 94 (2015); K. Medjanik et al Nat. Mater. 16 615 (2017); O. Fedchenko et al. New J. Phys. 21 013017 (2019).

[2] A. Damascelli et al. Rev. Mod. Phys. 75 473 (2003).

[3] T. Valla et al. Science 285 2110 (1999); C. L. Smallwood et al. Science 336 1137 (2012); G. Levy et al. Phys. Rev. B 90 045150 (2014); C. W. Nicholson et al. Phys. Rev. B 99 155107 (2019).

[4] G. Carleo et al. arXiv:1903.10563.

[5] R. P. Xian et al. Ultramicroscopy 202 133 (2019). Y. Yamaji et al. arXiv:1903.08060.