Dr. Georgios Exarchakis: 11.09.2019, 13– 13: 45 Uhr, Robert-Mayer-Straße 10, Raum 612

Solid Harmonic Wavelet Scattering: Predicting Quantum Molecular Energy from Invariant Descriptors of 3D Electronic Densities

We introduce a solid harmonic wavelet scattering representation, invariant to rigid motion and stable to deformations, for regression and classification of 2D and 3D signals. Solid harmonic wavelets are computed by multiplying solid harmonic functions with Gaussian windows dilated at different scales. Invariant scattering coefficients are obtained by cascading such wavelet transforms with the complex modulus nonlinearity. We study an application of solid harmonic scattering invariants to the estimation of quantum molecular energies, which are also invariant to rigid motion and stable with respect to deformations. A multilinear regression over scattering invariants provides close to state of the art results over small and large databases of organic molecules.

Dr.-Ing. Michael Götz: 11.09.2019, 14:45 – 15:30 Uhr, Robert-Mayer-Straße 10, Raum 612

From pictures to data-driven Precision Medicine with machine learning and context-information

Imaging methods like ultrasound, computed tomography (CT), magnetic resonance imaging (MRI) or digital microscopy are nowadays an integral part of clinical routine. With them, a huge amount of images are produced every but usually only visual inspected. However, these images are not only pictures but also data. If it is possible to extract the hidden information in images, they can be used to define subgroups within a disease. Based on the idea of precision medicine, a subgroup-specific treatment will then improve the treatment effect. Machine learning methods are powerful tools for this setting. However, applications of machine learning in the field of medical imaging face difficulties like missing or expensive annotations, noisy data or small training cohorts which hamper its use. To overcome these limitations, context information might be used for example the possible variation in the images, common or expected structures, additional clinical parameters of the patient, or images from other modalities. This opens the questions on how to incorporate such information and the resulting effects. This talk will show how context information and image fusion enables image-based precision medicine and what are current lines of research in this setting.