A versatile deep learning approach to generalize landmark positioning

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Despite the growing development of morphometric approaches based on deformable registration of 3D surfaces directly or indirectly via dense pseudo-landmark templates, landmark labelling of 3D objects remains a current and routine task in geometric morphometrics analyses. However, manual labelling is a tedious and time-consuming task, highly prone to intra-/inter-observer variability, requiring a high level of expertise, and is becoming incompatible with the increasing throughput of imaging technologies. Methods to automate the process have been developed, mainly based on the deformable registration of 3D images, surfaces or point-set. Whereas overall shapes are qualitatively well described with these algorithms, biases are observed in both the localization and the variance-covariance of landmarks. Some attempts using learning have been made to correct these biases but limited so far to specific anatomical parts of some organisms.

In this work, we aim at developing a versatile approach for learning landmark positioning that could be used to generalize an automated positioning of landmark not dependent of the vertebrate species and the specific skeletal element under study. The developed pipeline starts from an approximate prediction of landmarks obtained from a global registration of a reference model on the object, step which remains specific, and uses these predictions to subset the surface. The resulting local 3D surface is then parametrized in 2D and colorized to enhance some geometric features (ridges, flaws, hollows. . .) according to differential geometry and ambient lighting algorithms. The resulting images, quite generic of any bone structures, are associated to the manual landmark positions to train different Convolutional Neural Network (CNN) algorithms. Our results are promising with landmark predictions closer to the manual positioning than current deformable algorithms.

Automatic crater detection and classification using Faster R-CNN

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Planetary surfaces undergo continuous transformation driven by geological processes like volcanic eruptions and impacts. Understanding the distribution of impact craters is crutial to have a better comprehension of how planetary surfaces envolve through time (Hartmann & Neukum, Springer, 2001). This research project aims to develop a computer vision algorithm which automatically detect and classify craters from planetary surfaces images to create a comprehensive database encompassing crater positions, sizes, and their characteristics. The database will serve as a valuable resource for planetary scientists, facilitating the study of relative age, geological features distribution and so on, enabling a deeper understanding of planetary geological history and evolution.

For this work we use high-resolution planetary surface images from the Mars Reconnaissance Orbiter Context camera (CTX) which cover 99.5% of Mars (Dickson & al., LPSC, 2018). We also use an existing crater database listing over 376,000 craters of a size > 1 km in diameter (Lagain & al., Geological Society of America, 2021). Then, we train a Faster R-CNN computer vision algorithm on a subset of images and we tested it on a separate subsets. Our study demonstrated good results comparable to recent literature, achieving a mean average precision with an Intersection over Union criterion ≥ 0.5 (mAP50) > 0.8 (Benedix & al., Earth and Space Science, 2020 ; LaGrassa & al., Remote Sensing, 2023). Regardless of crater size, as long as it exceeds 10 pixels, the algorithm consistently performed well at every latitude (Martinez & al., PSS, under review).

Revealing polymer nanoobjects: AI Explores Impact of Block Size on morphology evolution

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Polymer nanoparticles are increasingly used in diverse fields ranging from nanomedicine, where they deliver drugs with precision, to cosmetics, enhancing product performance. Polymerization-Induced Self-Assembly (PISA) is an emerging technology that enables the versatile creation of nanostructures such as micelles and vesicles. Despite its potential, predicting the precise shapes of these structures remains challenging and usually involves complex and time-intensive experiments.

To streamline this process, we leverage Artificial Intelligence (AI), using supervised machine learning and deep neural networks to explore how variations in polymer structures influence the morphologies achieved by PISA. We train our models on carefully selected but limited datasets from existing literature, enabling them to predict phase diagrams for a broad range of polymer compositions. Our initial experiments have validated the accuracy of these predictions, confirming the robustness of our approach. Our research demonstrates AI's potential in unraveling complex PISA dynamics, promising significant advancements in this field.

Unlocking 3D nanoparticle shapes from 2D HRTEM images: classification and denoising at atomic resolution

Romain Moreau, Hakim Amara, Maxime Moreaud, Jaysen Nelayah, Adrien Moncomble, Christian Ricolleau, Damien Alloyeau, Riccardo Gatti Nanoparticles (NPs) are typically observed and analysed using High Resolution Transmission Electron Microscopy (HRTEM) for highly precise structural studies at the atomic scale. However, determining their 3D shapes from 2D HRTEM images is a tedious process. Indeed, this type of analysis is based on manual post-processing which suffers, among other issues, from experimental noise or human bias performed at post-experimental stage. In this context, the integration of artificial intelligence (AI) methodologies into data acquisition and analysis protocols is a very promising approach [1]. To tackle the problem of identifying the 3D shape of NPs, we developed a Deep Learning (DL) model to automate this task ensuring reliable statistical analysis of a large number of NPs many of which cannot be identified by conventional methods.

For this purpose, we extend an approach we had developed to identify the structure of carbon nanotubes from their Moiré patterns obtained from HRTEM images [2]. More precisely, the DL model, leveraging Convolutional Neural Networks (CNNs), is trained on datasets of simulated HRTEM images of NPs, labelled according to their shapes, ranging from 4 to 8 nm. A critical point of this study was generating a representative and optimised dataset. To accomplish this, we constructed atomistic 3D models of NPs deposited on an amorphous carbon substrate, subjecting NPs to random rotations to encompass all potential observed orientations. Furthermore, we simulated the amorphous substrate using realistic carbon membrane derived from a tight-binding framework and noise models, to mimic experimental conditions [3]. Finally, HRTEM images were simulated using the Dr Probe code [4] based on the multi-slice method with parameters consistent with aberration-corrected transmission electron microscopes.

The objective of generating an optimal training dataset was attained through comprehensive studies evaluating the impact of various parameters, including amorphous carbon, resolution, focusing conditions, NPs' size, and NPs' orientations, on DL model predictive accuracy. This approach has resulted in the development of an efficient and accurate DL framework for predicting 3D NP shapes from 2D HRTEM images, validated across both simulated and experimental datasets (see Figure 1).

However, when the contrast between the investigated nanoparticles and the substrate is highly degraded, performances may drop. Hence, we are currently training a Deep Learning (DL) model to automatically restore best nanoparticle-substrate contrast on acquired images. To this end a UNet-like model [5] has been trained on our simulated dataset [4] with patches procedure [6]. As shown on Figure 2, we have exhibited promising outcomes: across various regions of simulated HRTEM images under different defocusing conditions, the model demonstrates an ability to generate contrast close to the best achievable (ground truth).