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Fusing Online Gaussian Process-Based Learning and Control for Scanning Quantum Dot Microscopy

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Scanning quantum dot microscopy is a technique for imaging electrostatic surface potentials with atomic resolution. To this end it uses a sensor molecule, the so-called quantum dot (QD), which is bonded to the tip of a frequency modulated non-contact atomic force microscope. The QD is moved in the vicinity of the surface atoms so that it experiences the surface potential. By superimposing an external potential using a tip-surface bias voltage V_b, the QD's potential is modulated to reach critical values at which the QD changes its charge state. In consequence to these charging events, the tuning fork's oscillation frequency f changes abruptly, making the charging events appear as dips in the so-called spectrum $\Delta f(V_b)$, characterized by the positions $V^{\mp}$ of their respective minimum points. These dip positions $V^{\mp}$ are used for reconstructing the surface potential image.

While scanning the sample in a raster pattern, $V^{\mp}$ change with the position of the dip in consequence of the sample topography and its electrical properties. To efficiently and reliably track $V^{\mp}$ we have employed a two-degree-of-freedom control paradigm within which a Gaussian process and an extremum seeking controller are used. The Gaussian process is employed in the feedforward part to compute a prediction of $V^{\mp}$ for the next line based on the data of previous lines. This prediction is thereafter applied pixel by pixel as initial point to the extremum seeking controller, which is used in the feedback part to correct deviations between the prediction and the true value. Obtaining an accurate prediction is hereby critical for correct operation as the extremum seeking controller is only capable of tracking $V^{\mp}$ as long as the current value V_b is within the dip. For reducing the computation time in order to make the controller suitable for utilization in practice, we have implemented and tested different approximation approaches for sparse GP implementation.

In simulative testings, we have shown that using the proposed two-degree-of-freedom control para-digm results in shorter scan times while achieving a high image quality when compared to feedback control only. The most promising approximation approach for sparse GP implementation regarding scan time and image quality has been found to be the fully independent training conditional approximation. We have further shown that its computation is sufficiently low for usability in practice.

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