Atomic Super-Resolution Tomography

Poulami Somanya Ganguly[1, 2], Felix Lucka[1, 3], Hermen Jan Hupkes[2], Joost Batenburg[1, 2]

[1] Centrum Wiskunde & Informatica, Amsterdam, The Netherlands; [2] The Mathematical Institute, Leiden University, Leiden, The Netherlands; [3] Centre for Medical Image Computing, University College London, London, United Kingdom

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Live poster - https://poulamisganguly.github.io/poster_IS20/

Introduction

Electron tomography is a technique for resolving the interior of nanomaterials from a series of projection images. **Discrete tomography** approaches have been shown to reconstruct nanocrystals of increasing complexity. A key limitation of these methods is that they assume atoms to lie on a coarse spatial grid whereas, in practice, **lattice defects** in nanocrystals cause atoms to deviate from regular positions.

We present two alternative **grid-free** reconstruction approaches: 1) a super-resolution approach that allows for continuous deviations of atom locations, and 2) a **deep learning** approach to identify atom locations from blurred reconstructions

Summary of Main Results

1. Allowing for continuous deviations of atom locations **aids reconstruction** of test lattices with data from **very few tilt angles** (2 or 3).
2. Incorporating a physical model for the **potential energy of the atomic configuration** corrects for **poor initialisations**.
3. **Learned post processing** from reconstructed images performs poorly for limited data.

Mathematical Formulation

An atomic configuration is characterised by a positive measure μ on a bounded subset X of $\mathbb{R}^d$, which represents the electron density. The Radon transform of the measure, $\mathcal{R}\mu$, provides a simplified mathematical model of the image formation process. The corresponding inverse problem is to recover μ from noisy observations given by $y = \mathcal{R}\mu + \varepsilon$.

We consider atomic configurations to be **sparse measures** of the form: $\mu = \sum_{i=1}^{n} w_i (G * \delta_{\boldsymbol{x}_i})$, where G denotes a Gaussian that quantifies thermal motion of atoms and the weights w_i are used to differentiate between atom types.

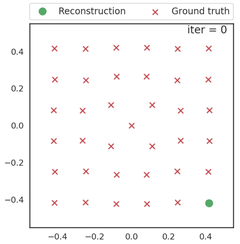
To recover μ, we model interatomic interactions explicitly by the **Lennard-Jones** pair potential and solve the following optimisation problem:

$$\underset{\boldsymbol{x}\in\mathcal{C}, w\in\{0,1\}^n}{\text{minimise}} \quad \Big\| \sum_{i=1}^{n} w_i \mathcal{R}(G * \delta_{\boldsymbol{x}_i}) - y \Big\|_2^2 + \alpha V_{\text{tot}}(\boldsymbol{x}),$$

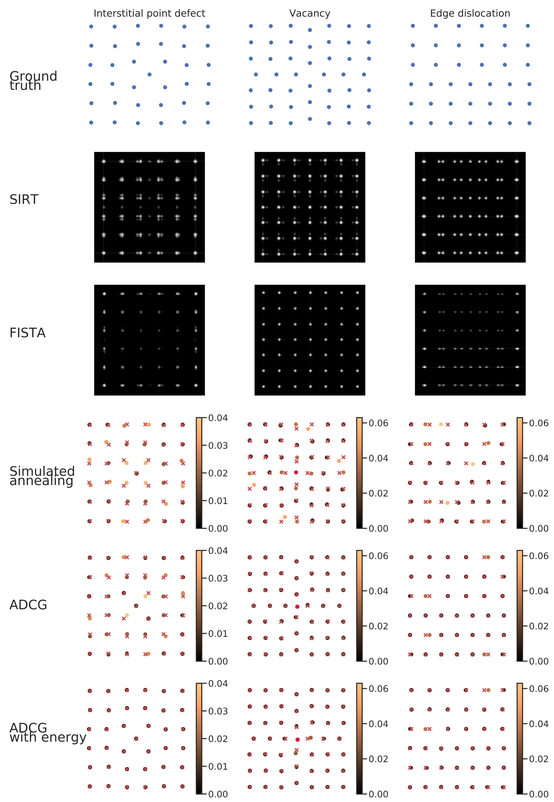
where V_{tot} is the total potential energy and α is a regularisation parameter.

Results

We used a modified version of the **alternating descent conditional gradient (ADCG)** (Boyd, Schiebinger, and Recht 2017) algorithm to obtain atom locations. At each iteration, the algorithm 1) **adds a new atom** on a coarse grid and 2) **locally moves** all atoms. An animated reconstruction run is shown on the right.

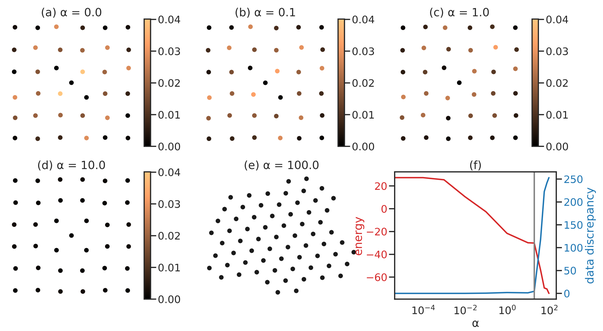


Comparison of reconstructions



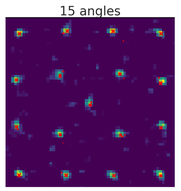
Reconstructions of common lattice defects from 2 projections. For simulated annealing, ADCG ($\alpha = 0$) and ADCG with energy ($\alpha > 0$) reconstructions, atoms are coloured according to their Euclidean distance from the ground truth. The ground truth positions are marked with red crosses.

Effect of adding energy



Tuning α amounts to moving from data-optimal to energy-optimal configurations. Increasing α beyond an optimal value (grey line in plot) leads to a large increase in the data discrepancy due to addition of more atoms.

Learned Post-processing



We trained a deep neural network (Boyd et al. 2018) to identify atom locations from blurred SIRT reconstructions.
This approach although more scalable than ADCG did not perform well for cases where data from only very few angles were available. SIRT reconstructions with identified atoms (red crosses) are shown on the left.

Outlook

- Incorporate appropriate features of global optimisation into ADCG
- Use more realistic potential energy models
- Explore deep learning based iterative schemes

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References

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