Atomic Super-Resolution Tomography

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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.

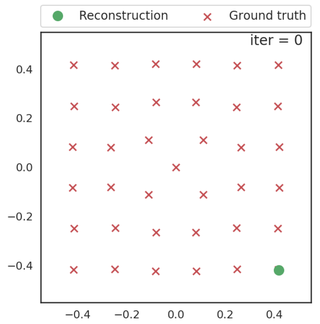
To recover μ, we model interatomic interactions explicitly by the **Lennard-Jones** pair potential and solve the following optimisation problem:

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

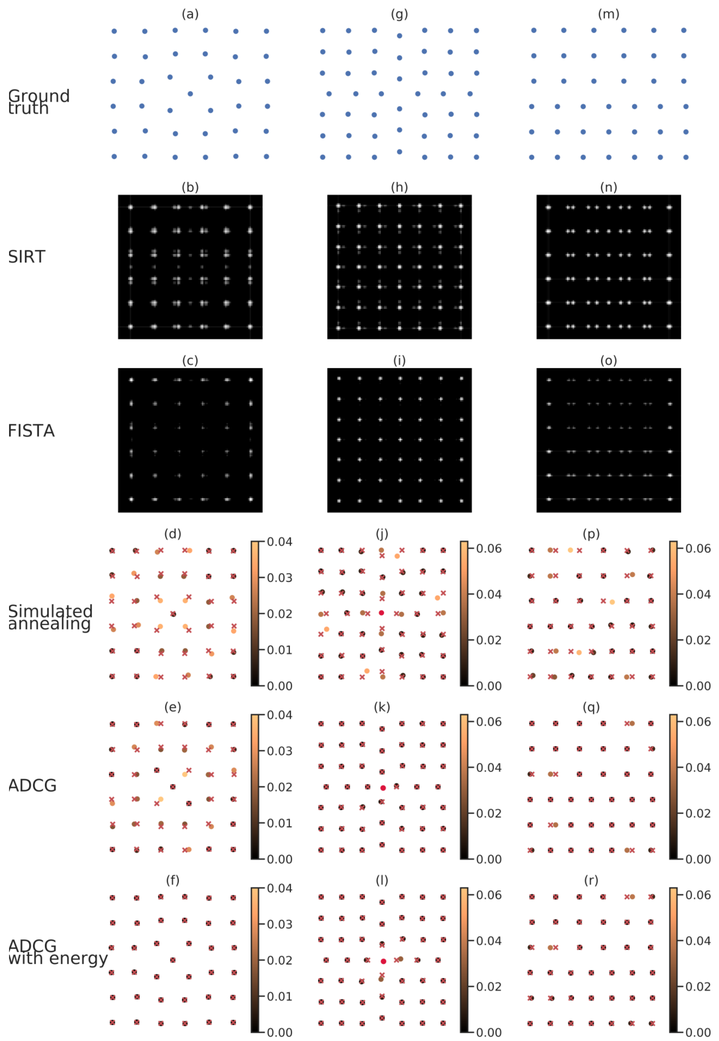
where V_{tot} is the total potential energy and α is a regularisation parameter.

Results

We used a modified version of the **alternating descent conditional gradient (ADCG)** 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.

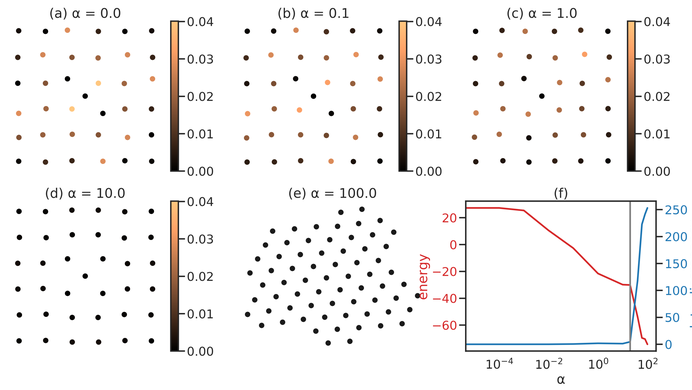


Comparison of reconstructions



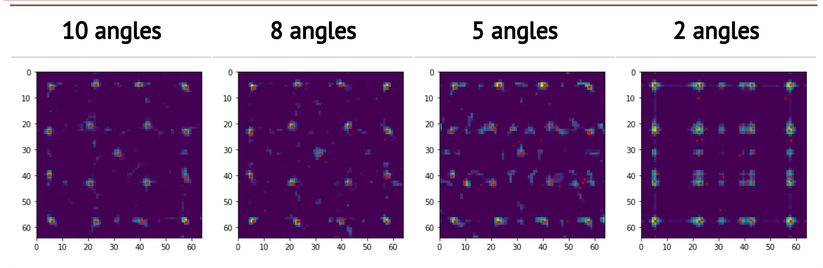
Reconstructions of common lattice defects from 2 projections. For simulated annealing, ADCG ($\alpha = 0$) and ADCG with energy ($\alpha > 0$) reconstructions, atoms are coloured according to their Euclidean distance from the ground truth. The ground truth positions are marked with red crosses.

Effect of adding energy



Tuning α amounts to moving from data-optimal to energy-optimal configurations. From the plots of potential energy and data discrepancy, an optimal value of α (indicated by the grey line) is selected. Increasing α beyond this optimal value leads to a large increase in the data discrepancy due to addition of more atoms.

Learned Post-processing



Outlook

- Incorporate appropriate features of global optimisation into ADCG
- Use more realistic potential energy models
- Explore deep learning based iterative schemes to scale up to real electron tomography data

References

Acknowledgements

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement no. 765604.