Sparsity-based algorithms for inverse problems
Ganguly, P.S.

Chapter 6

Conclusion

In this thesis we investigated ways to leverage sparsity in the design of practical algorithms for various inverse problems. The inverse problems we focused on arose in quite different application areas, with each being a topic of intensive research in its own right. The methods presented in this thesis, while being tailored to each application, also share some overarching similarities in design and implementation. This, we believe, indicates the importance of developing mathematical tools that can be applied to more than one practical problem.

In this concluding chapter, we summarize the contributions of this thesis and point to some future research directions.

In Chapter 2 we presented a filter-optimization method to improve reproducibility of reconstructions for synchrotron tomography. Our method used sparsity in the design of optimal filters. By using the fact that many standard real-space filters taper off to zero at the detector boundaries, we were able to reduce the number of filter coefficients that need to be computed. These sparse-basis filters, when optimized to various implementations of direct reconstruction algorithms, were shown to result in reconstructions with fewer differences than those that were obtained with standard filters. Our work in this chapter is a stepping stone towards a more reproducible synchrotron pipeline, which will require both hardware and software modifications.

In Chapter 3, we demonstrated the use of sparsity in reconstructing atomic defects. We built on existing ideas of grid-free sparse optimization to propose a more canonical discretization of the atomic-resolution reconstruction problem. This discretization did away with the need for reconstructing on a voxel grid. Instead, we modelled atomic configurations as sparse measures, allowing for continuous deviations of atomic locations. We showed how, coupled with physical prior knowledge on the potential energy of atomic configurations, our grid-free method is able to reconstruct common lattice defects with very few projections. We demonstrated the power of our approach in proof-of-concept numerical studies, and proposed further modifications that would make our algorithm applicable to real data.

We extended our grid-free sparse optimization method to investigate marker-based alignment for cryoET in Chapter 4. Here we modelled marker configurations as deforming measures and used similar ideas to those first developed in Chapter 3 to solve for marker locations and deformations. We applied our approach to synthetic data as well as real data of markers embedded in ice. Our numerical experiments showed that this approach was able to localize markers without the need for the user to label markers in projection data, a cumbersome and error-prone pre-processing task that is needed for existing methods. Our approach is flexible and allows for different models of sample deformation and marker shapes.

In Chapter 5, we used sparsity to recover pairwise interactions that lead to network formation in vertebrates. Our work builds on existing literature on nonlinear equation learning, where a sparse combination of library terms is learnt for time-series data. We used particle-based simulations of angiogenesis to generate time-series data of interacting cells, and were able to recover the relevant interaction terms that led to the formation of networks. Our work is a stepping stone to learning interaction terms in settings where these are not evident, such as other simulation paradigms like the cellular Potts model and experimental data of vascular network formation from endothelial cells.

The work in this thesis shows how sparsity can be used both implicitly and explicitly. Examples of the former include choosing sparse filter basis functions and making certain algorithmic choices, such as adding only one atom to the current solution at each iteration. An explicit way to include sparsity while solving inverse problems is to include an ℓ^1 regularization term in the objective, for example when inferring pairwise interactions between cells.

One promising paradigm developed in recent years is to parametrize the regularizer with a neural network. In the case of tomographic imaging, such learned regularizers [117], [118] have been shown to outperform methods with hand-crafted regularization terms. This is part of a wider interest in the application of data-driven approaches to inverse problems [56], [119]. Although learned approaches might be superior to several classical approaches that enforce sparsity explicitly, ideas of sparsity are also important for improving the efficiency and robustness of deep-learning methods. One example is the use of sparsity to reduce the complexity of deep neural networks by pruning network weights. This has been shown to result in more generalizable networks that also use less resources to train [120]. Another example is using sparsity implicitly in choosing an appropriate discretization for the studied system. This approach is similar to our work on reconstructing nanocrystal defects, and has recently been used to study the problem of atomic-resolution cryo-electron microscopy of proteins [121]. Such examples indicate the continued relevance of sparsity-based approaches in designing efficient algorithms for inverse problems.