

Assignment 2

Due date: Wednesday, March 7

A generalization of RRR

Consider the following generalization of RRR,

$$\dot{x} = P_A((1 + \gamma)P_B(x) - \gamma x) - P_B((1 - \gamma)P_A(x) + \gamma x),$$

where $\gamma > 0$ is a parameter. Using the same method of analysis used in lecture for $\gamma = 1$, show that the flow in the neighborhood of a solution is changed in only a minor way. As before, model the constraint sets A and B as

$$\begin{aligned} A &= \tilde{A} + c_A \\ B &= \tilde{B} + c_B, \end{aligned}$$

where $\tilde{A}, \tilde{B}$ are linearly independent subspaces and c_A, c_B are in the orthogonal complement of their span. You should find attraction to a hyperplane of fixed points for the feasible case, $c_A = c_B$, and monotone flow away from the non-solution when $c_A \neq c_B$.

He who must not be retrieved

By a stroke of luck we are in possession of diffraction data taken of the math wizard who appropriated the term “phase retrieval” for his own line of research that has had no relevance for scientific phase retrieval. Look for `DarkLordData` in the data directory of our github site. Use RRR with the standard projections for phase retrieval with a fixed support constraint to reconstruct his image.

This is a warm-up exercise for the much harder form of phase retrieval featured in the next problem.

Crystallographic phase retrieval

It is relatively straightforward to adapt the method you used to solve the previous problem — phase retrieval with a fixed support constraint — to the case of crystals. Because the signal (electron density) in a crystal is truly periodic, its support in the computational grid (in FFT computations) does not have any of the restrictions we apply to an isolated object: the entire grid is the crystal’s unit cell. However, a prior constraint is still needed to retrieve the phases. This takes the form of a constraint

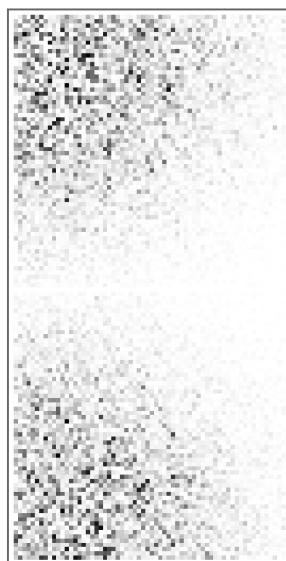
on the *size* of the support. In other words, we do not know *where* in the unit cell the atoms are, but we know how little space they occupy.

A constraint on the size of the support is also called a sparsity constraint. Consider a real-valued signal ρ on N pixels/voxels. Find an algorithm that computes the projection $P_{|S|}(\rho) = \rho'$ to the nearest signal ρ' that is non-zero on at most $|S|$ of the pixels/voxels. What modification is needed for the projection $P_{|S|+}(\rho) = \rho'$, where ρ' is also required to be non-negative?

Use $P_{|S|+}$ together with the usual Fourier magnitude projection to reconstruct the easiest benchmark instance of crystallographic phase retrieval:

<https://github.com/veitelser/phase-retrieval-benchmarks/blob/master/data/data100E>

The benchmarks are synthetic (made-up) 2D crystals with 128×128 pixels in the unit cell (easier to render than 3D crystals). When you open the data file above you will see a 128×64 array of integers:



0	41	...	11	14
93	586	...	2	53
126	226	...	12	5
78	961	...	11	44
...	...	...	...	...
0	0	...	0	0
...	...	...	...	...
78	125	...	10	3
126	617	...	0	17
93	303	...	0	9

These are simulated photon counts, so to get the Fourier magnitudes you need to take their square roots. The other half of the array of intensities is determined by $|\hat{\rho}(-q)| = |\hat{\rho}(q)|$ (since ρ is real). The counts on row 65 and column 65, at the outmost edge of the diffraction pattern, are all zero.

Note that the data file has zero photon counts for $q = (0, 0)$, at the upper left-hand corner. This corresponds to the fact that the forward-scattered photons cannot be detected and so there is no measurement of that Fourier magnitude. We therefore

have no constraint on $\hat{\rho}(0, 0)$ and the Fourier magnitude projection has to be modified to simply leave this Fourier coefficient unchanged.

If your reconstruction succeeds, you should see 50 small atoms and 50 large atoms. Atoms take up on average 8 pixels each, so you should set $|S| = 800$. The reconstruction error $\|p_1 - p_2\|$ will never become exactly zero because the finite photon counts introduce noise.