

An Introduction to Phase Retrieval

For some function f on a 2D or 3D space Ω , if we perform the Fourier transform, then we obtain:

$$F(k) = \int_{x \in \Omega} f(x) e^{-2\pi i x k} dx = |F(k)| e^{i\psi(k)}$$

The norm $|F(k)|$ is called the magnitude and the angle $\psi(k)$ is termed the phase. Suppose we are given the magnitude and phase, then for any f in the Schwarz space, there is a bijective function F being its Fourier transform, and f is also F 's unique inverse Fourier transform. That is, given both magnitude and phase, we can perfectly recover the original function.

However, what if the phase information is lost? Apparently this problem is no longer well posed, since there exists F in the reciprocal space, the space of Fourier transform, such that more than one function in the real space have the same Fourier transform F . With appropriate constraints, it is possible to reconstruct the phase information, usually with the aid of iterative methods.

However, why would we be interested in the problem of phase retrieval? It turns out that this problem has played an important role in many fields including X-ray crystallography and lensless imaging.

X-ray crystallography is the study of using X-ray beams incident on crystal molecules to create diffraction patterns. When a beam of X-ray, which is wavelike in the molecular level, is incident on crystal molecules, diffractions occur and thus lead to a new pattern in the detector. Essentially,

the data that we can gather is the magnitude of the Fourier transform of the electrons' density. If the electrons' density can be revealed then a lot of useful information, such as molecular structure, chemical bonds, etc, can be unveiled. Therefore, we have reduced the original problem to the phase retrieval problem.

Unlike the ill-posed problem mentioned before, the practical problem usually comes with more constraints to the phase. For example, certain symmetries are available for particular objects.

So, how can we solve the phase retrieval problem? In general, the most general case remains open, despite the efforts of mathematicians and scientists over more than four decades. A lot of the partial results, however, are available, and has great value in applications. Here we will review two iterative methods: error reduction (ER) and hybrid input-output (HIO), based on which most methods are proposed.

1 Error Reduction

ER is due to Gerchberg and Saxton. The essential idea is to alternate between two operators P_S and P_M .

To start, we randomly generate an initial phase $\tilde{\psi}(k)$. Along with the random phase, we use the magnitude $|F(k)|$ to construct an initial guess $\hat{F}_1(k) = |F(k)|e^{i\tilde{\psi}(k)}$. Perform an inverse transform to obtain $\rho_{(1)}$, our initial guess of the density.

Now consider the support projector P_S . For the density, we have prior knowledge that only in the support S would the density be nonzero. Hence, we define the support projector as

$$P_S(\rho) = I_S(\rho)$$

where I_S is simply the delta function on S . The other projector is the modulus projector P_M ,

defined by,

$$P_M = \mathcal{F}^{-1} \circ \tilde{P}_M \circ \mathcal{F}$$

where \mathcal{F} is the Fourier transform and \tilde{P}_M is defined by

$$\tilde{P}_M(\hat{F}(k)) = \tilde{P}_M|\hat{F}(k)|e^{i\hat{\psi}(k)} = |F(k)|e^{i\hat{\psi}(k)}$$

That is, we first perform a Fourier transform to get the reciprocal space data, and then replace the magnitude by the true magnitude that we gathered at the beginning.

The iterative scheme is:

$$\rho^{(n+1)} = P_M P_S(\rho^{(n)})$$

Intuitively, we first erase those densities that should not exist, and then perform Fourier transform, and adjust the magnitude. This approach would require the support to be relatively small compared to the whole real space Ω .

2 Hybrid Input-Output

The HIO uses the two projectors mentioned above but is defined differently:

$$\rho^{(n+1)}(x) = \begin{cases} P_M \rho^{(n)}(x) & \text{if } x \in S \\ (I - \beta P_M) \rho^{(n)}(x) & \text{if } x \notin S \end{cases}$$

where I is the identity mapping and β is the feedback parameter, usually chosen to be 0.9.

HIO can be combined with ER: for example, we can repeat a procedure consisting of 20 HIO followed by one ER. This usually has a better effect than either method alone.

However, for both methods, a practical problem is that we need to know the support exactly. In most real-life scenarios, this requirement cannot be fulfilled. Marchesini et al. proposed a way to determine the support iteratively, the shrinkwrap algorithm. Basically the shrinkwrap algorithm

uses an initial guess that is big enough to cover the real support, and then set some pre-fixed threshold value to filter out the points not in the support. This approach sometimes suffer from over-shrinking.