Maximum-likelihood absorption tomography

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Abstract. – Maximum-likelihood methods are applied to the problem of absorption tomography. The reconstruction is done with the help of an iterative algorithm. We show how the statistics of the illuminating beam can be incorporated into the reconstruction. The proposed reconstruction method can be considered as a useful alternative in the extreme cases where the standard ill-posed direct-inversion methods fail.

Introduction. – The standard reconstruction method in present computerized tomographic (CT) imaging is the filtered back-projection (FBP) algorithm which is based on the Radon transformation [1]. Unfortunately FBP fails in case of missing projections and/or if strong statistical fluctuations of the counting numbers are present in the small detector pixels. The latter situation occurs e.g. in neutron tomography [2], if monochromatic neutron beams are applied in order to avoid beam artifacts [3] or at the investigation of strong absorbing materials. The cases of missing projections and incomplete data sets for monochromatic neutron beams have been already investigated in the past in detail by means of algebraic reconstruction technique [4, 5]. Scattering data from a double crystal diffractometer have been used to reconstruct 2D scattering pattern and the results were compared with the standard FBP. With this algebraic approach one could reconstruct 2D pattern in spite of the lack of nearly 90 degrees of the scanning angle, whereas in such cases the FBP method entirely failed. The computing time, however, was extremely long (up to several hours), so that this method is useful for rather small 2D arrays (100 x 100 pixels) only.

The new reconstruction method proposed in this paper can improve several tomographic applications in neutron optics which in many cases are limited by the weak intensity and the poor detector resolution. The use of well collimated pencil beams which are scanned across the sample surface could dramatically enhance the spatial image resolution but this method is only rarely used due the long measurement times [6]. An improved reconstruction method can encourage new applications in neutron optics which often suffer from the low counting

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numbers. Generally the new algorithm can achieve better reconstruction results or reduce the scanning time in neutron optics and in medical and biological CT imaging.

LinPos tomography. — Basic notions and the geometry of experimental setup are as follows. Let us assume that the sample is illuminated by parallel monochromatic pencil beams, see Fig. 1. Data consist of the number of particles counted behind the sample for $M$ different scans – each scan being characterized by horizontal position $h$ and rotation angle $\varphi$. Alternatively, a broad illuminating beam combined with a position-sensitive detector (CCD camera) placed behind the sample can be used. In that case $h$ labels pixels of the camera. For the sake of simplicity a collective index $j \equiv \{h, \varphi\}$ will be used, hereafter, to label the scans.

Mean number $\bar{n}_j$ of particles (intensity) registered in $j$-th scan is given by the exponential law

$$\bar{n}_j = \bar{n}_0 \exp\left(-\int \mu(x, y) ds_j\right), \tag{1}$$

where $\bar{n}_0$ is the intensity of the incoming beam, $\mu(x, y)$ is the absorption index (cross section) of the sample in position $\{x, y\}$, and the integration is the path integration along the pencil beam. This exponential attenuation law is a good approximation if scattering can be neglected. The beam hardening artifacts would also modify Eq. (1) but this complication can be avoided experimentally by the use of monochromatic beams \[6\]. For practical purposes, it is convenient to discretize Eq. (1) as follows,

$$\bar{n}_j = \bar{n}_0 \exp\left(-\sum_{i=0}^{N} \mu_i c_{ij}\right). \tag{2}$$

The sample is now represented by a 2D mesh. Each cell is assumed to have a constant absorption index. The variables are now $N$ numbers $\mu_i$ specifying absorption indices of those cells. Overlaps between beams and cells are stored in the array $\{c_{ij}\}$, see Fig. 2.

Let us first ignore the statistics of the illuminating beam, and assume that the counted numbers of particles $\{n_j\}$ do not fluctuate, $n_j = \bar{n}_j$, $\forall j$. Taking logarithms of both sides of Eq. (2), one obtains a system of $M$ linear algebraic equations for $N$ unknown absorption coefficients $\mu_i$:

$$f_j = p_j, \quad j = 1 \ldots M, \tag{3}$$
where we defined,
\[ f_j = -\ln \frac{n_j}{n_0}, \quad p_j = \sum_i \mu_i c_{ij}. \] (4)

Notice that problem (3) is a linear and positive (LinPos) problem. Positivity follows from the fact that no new particles are created in the sample. Although direct inversion of Eq. (3) is possible for \( N \geq M \), the solution is not always positively defined. A negative value of a reconstructed \( \mu_i \) would suggest that particles were being created in the \( i \)-th cell in the course of the experiment, which would obviously be a wrong conjecture. This problem can be avoided if the problem (3) is solved in the sense of maximum likelihood (ML) on the space of physically allowed absorption coefficients. In this approach one considers the data \( f \) and the prediction of the theory \( p \) as two probability distributions. One looks for absorption coefficients \( \{\mu_i\} \) that minimize the Kullback-Leibler “distance”
\[ d(f, p) = -\sum_j f_j \ln \frac{p_j}{f_j} \] (5)
between the data \( f \) and the theory \( p \). Here a little extra care is needed since \( p \) and \( f \) are generally not normalized to unity. The minimum of the Kullback-Leibler distance corresponds to the maximum of the maximum likelihood (ML) functional [11]
\[ \mathcal{L} = \prod_j \left( \frac{p_j}{\sum_k p_k} \right)^{f_j}, \] (6)
that quantifies the likelihood of the given distribution \( \{\mu_i\} \) in view of the registered data. We seek the maximum-likely distribution of the absorption indices. A convenient way how to find it is the celebrated Expectation-Maximization (EM) iterative algorithm [12, 13],
\[ \mu^{n+1} = R(\mu^n) \cdot \mu^n, \] (7)
where
\[ R_i = \frac{1}{\sum_j c_{ij}} \sum_j \frac{f_j c_{ij}}{p_j(\mu)}, \] (8)
and \( \mu^0 \) is some initial strictly positive distribution \( \mu_i^{(0)} > 0, i = 1 \ldots N \). A nice feature of EM algorithm is that its convergence is guaranteed for any input data \( f_j \) [14]. For this reason it became a valuable tool in many inverse problems which can be reduced to the form of Eq. (3), e.g. in positron emission tomography [14–16]. The original derivation of EM algorithm is based on alternating projections on specially chosen convex sets of vectors. However, one could directly use the calculus of variations to derive the necessary condition for the extreme of the functional [13]. Iterating these, one eventually arrives at the EM algorithm again. An advantage of this alternative derivation is that it can be also applied to more realistic physical models of the actual absorption experiment. One such possible generalization will be studied in the following section.

**Tomography with Poissonian signals.** — Real signals are not composed of a sharp number of particles. For instance, two signals often used in experiments — beam of thermal neutrons and laser light — both exhibit Poissonian fluctuations in the number of particles. Also monochromatic neutron beams are correctly described by Poissonian statistics if the detected count events occur mutually independently [17]. The knowledge of the true character of signal illuminating the sample is a useful piece of prior information, which can be utilized for improving the performance of ML tomography.
As the Poissonian character of the signal is preserved by the process of attenuation, the counted numbers of particles behind the sample are random Poissonian variables. The corresponding likelihood functional reads,

$$ L \propto \prod_j \bar{n}_j^{n_j} e^{-\bar{n}_j}. $$

(9)

This is the joint probability of counting \( \{n_j\} \) particles. Mean values \( \{\bar{n}_j\} \) obey the exponential law (1) as before. They depend on the absorption in the sample \( \{\mu_j\} \) that is to be inferred from the data. The necessary condition for the extreme of the likelihood (9) can be derived using the calculus of variations. The extremal equation can be shown to have the same vector form as the extremal equation of the LinPos problem (8). The vector \( R \) now becomes

$$ R_i^{(\text{Poisson})} = \frac{\bar{n}_0}{\sum_j c_{ij} n_j} \sum_j c_{ij} \exp(-\sum_{i'} \mu_{i'} c_{i'j}). $$

(10)

When the input intensity \( \bar{n}_0 \) is not known, it can be estimated together with the absorption of the sample:

$$ \bar{n}_0 = \frac{\sum_j n_j}{\sum_j \exp(-\sum_i \mu_i c_{ij})}. $$

(11)

Poissonian tomography is intrinsically a nonlinear problem. This has serious consequences for the convergence properties of the iterative algorithm (7) and (10). Instead of converging to a stationary point it might end up in oscillations. Typically such convergence problems arise in the presence of very noisy data. When this happens, one can always decrease the length of the iteration step as follows: \( R_i \rightarrow R_i^\alpha \), \( i = 1 \ldots M \), \( 0 < \alpha < 1 \). Of course, any solution to the regularized problem is also a solution to the original problem.

**Discussion.** Generally, the reconstructed image will depend on which ML method is chosen to process the data; see the apparent difference between Eqs. (8) and (10). It is interesting to look more closely at the origin of this difference. Consider a tomographic setup with a Poissonian beam. Then the Poissonian algorithm should provide a better reconstruction than the LinPos algorithm which have been derived under the assumption of non-fluctuating signals. The LinPos reconstruction consists in minimizing the Kullback-Leibler distance between the data \( f \) and theory \( p \). When logarithms of the counted numbers of particles are chosen to be the input data rather than counted data itself, one arrives at the EM algorithm (8) and (10). Taking logarithms of actual data makes the problem linear and considerably simplifies the reconstruction. However, one could, instead, directly minimize the Kullback-Leibler distance between the counted data \( n_j \) and the corresponding theory \( p_j' = n_0 \exp(-p_j) \). Interestingly enough, the extremal equations associated with this variational problem are the same as Eqs. (8) and (10) derived above from the Poissonian theory (9). Choosing \( n_j \) instead of \( f_j \) as the data is equivalent to taking the Poissonian statistics of the signal into account! The difference between the LinPos and Poissonian ML reconstructions can thus be traced down to whether the measured data are used directly or not. Tampering with data prior to reconstruction may speed up and facilitate the whole process of reconstruction but some information about the object might get lost.

**Comparison with standard methods.** In a real experiment there are many factors that could influence the quality of the measured data and therefore also on the result of the tomography. Misalignments present in the experimental setup, instability of the illuminating beam,
white spots and damaged detector pixels can be such factors, to name a few. To avoid this problem we replaced the experiment by a simulation. The data were generated on a computer. The artificial object used in the simulation is shown in Fig. 3. The object is a circle made of a homogeneous material with many small round holes drilled through it. One additional rectangular piece of material was removed from the circle to make it less symmetric. Absorption index of the material was chosen in such a way that the maximum attenuation along a beam was close to 50% of the input intensity.

In the simulation, the object was subject to five different experiments. Their parameters are summarized in Table I. First four experiments correspond to the ideal situation of a very high beam intensity where the Poissonian detection noise can safely be ignored. The last reconstruction simulates more realistic conditions with 2000 counts per pixel in the open beam. Notice that a relatively small number of rotations is chosen for all five experiments. In this regime the Radon transformation is expected to yield bad results and the improvement of the maximum-likelihood tomography upon the standard technique should be most prominent. This regime is also important from the practical point of view. Doing more rotations implies a longer measurement time and more radiation absorbed by a sample. The latter may be an important factor if the imaging of biological samples is considered. So, imaging costs and damage done to a sample due to radiation might be reduced provided the improvement of the reconstruction technique gives comparable resolution with less data.

Reconstructions from the simulated data are shown in Figs. 4 and 5. The simulated data were first processed using the IDL imaging software (Research Systems Inc.) which implements the standard FBP algorithm (Radon transform), see Fig. 4. This software is one of the industrial standards in the computer assisted tomography. The same data were then processed using our iterative algorithm based on the maximization of the Poissonian likelihood function, see Fig. 5. In the absence of noise, see cases (a)-(d), the fidelity of a reconstruction depends on two main factors—the spatial resolution of the detector, and the number of rotations used. It is apparent from Figs. 4 and 5 that the latter factor is more

| reconstruction | angles | pixels | intensity |
|----------------|--------|--------|-----------|
| a              | 13     | 161    | ∞         |
| b              | 19     | 101    | ∞         |
| c              | 20     | 101    | ∞         |
| d              | 7      | 301    | ∞         |
| e              | 15     | 161    | 2000      |

Table I – Quality of the input data. The last column shows the mean number of counted particles per pixel in the incident beam.
Fig. 4 – IDL reconstructions from the simulated data, for parameters see Tab. I.

Fig. 5 – ML reconstructions from the same data. The proposed iterative algorithm, Eqs. (7) and (10), has been used for reconstruction.

important of the two. Very small number of angles cannot be compensated by an increased spatial resolution of the detector, compare e.g. cases (c) and (d), and reconstruction (d) is by far the worst one. However, ML tomography is much less sensitive to the number of angles than the standard filtered back-projection. Even the large rectangular hole in the object is hardly perceptible in Fig. 4d whereas it nicely shows in the ML reconstruction Fig. 5d. ML reconstructions are superior to the standard ones also in cases (a)-(c); notice that the reconstruction Fig. 5c done with as few as 20 different angles is nearly perfect.

Benefits of the ML tomography are fully revealed when the detected data are noisy. This is case (e) in Tab. I. Standard filtered back-projection applied to noisy data faces serious difficulties. This is due to ill-posedness of the Radon transformation where data are integrated with a singular filter function. Obviously such deconvolution greatly amplifies any noise present in the data. Having little or no prior information about the object it is difficult to tell true details of the object from artifacts. ML tomography gives much better results. Since noises are incorporated into the algorithm in a natural and statistically correct way artificial smoothing is not needed. Notice in Fig. 5e that noisy data yield a little distorted but otherwise clear image unlike the corresponding very noisy standard reconstruction shown in Fig. 4e. This is a nice feature of the intrinsically nonlinear ML algorithm which, in the course of reconstruction, self-adapts to the registered data and always selects the most likely configuration.

Finally let us emphasize that apart from the size of the reconstruction mesh $N$ there are no free parameters left in the ML algorithm to play with. This prevents one from interfering when the reconstructed image “looks bad.” This also makes the whole procedure more objective, which is a necessary presumption for the investigation of ultimate limits of reconstruction schemes.

Conclusion. – We presented a new reconstruction method for CT imaging based on the iterative maximization of the Poissonian likelihood. For small number of scans and/or short measurement time this method was shown to yield a significant improvement upon the standard filtered back-projection algorithm. This could be important for CT imaging with low-intensity beams, and for applications where strong irradiation of a sample during the scanning should be avoided. One area where reconstruction techniques of the type discussed in this
paper would be very useful are coherent reconstruction techniques such as interferometric phase tomography with X-rays [19, 20] or neutrons [21], or neutron holography [22]. There is hopefully more to come.

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