OPTIMAL SPECTRAL DECONVOLUTION OF INTERFEROGRAM SAMPLES

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1. INTRODUCTION

It is recognized that interferometers can give radiance estimates in the atmosphere at a much higher spectral resolution than that of current filter radiometers. The consequences can be the improvement of the retrieval of temperature and humidity profiles from radiance data as far as vertical resolution is concerned.
Some papers appeared in the literature concerning the optimization of the design of interferometers, as far as both the experimental equipment and the data to be measured are concerned (see, e.g., Revercomb et al., 1988, Amato et al., 1991). In particular much is known about the length of the measured interferogram. However some work has to be done in order to process the measured interferogram in an optimal way from the mathematical point of view. In fact some current techniques do not take account of the experimental error affecting the interferogram properly: they are based on the use of a *spectral window* whose size is fixed and in particular does not fit the experimental error (see Jenkins and Watts, 1968 for a review). In addition, other techniques, non linear in general, loose the nice computational properties of the original problem, namely the possibility to use FFT, and then do not seem to be advantageous for real-time applications (see, e.g., Amato et al., 1991).

Aim of the present paper is to introduce an optimal mathematical technique for retrieving the spectrum from an interferogram with the following features:

a) involve the use of FFT from a computational point of view, so that its speed can allow real-time applications with large quantities of data;
b) take account of the experimental error affecting the interferogram, in the sense that the amount of error present is recognized and the right amount of smoothing is applied;
c) must generate a final algorithm; this means that any step of the procedure is to be performed by the algorithm, without any external intervention of the researcher, so to give a true *objective* mathematical technique.

The algorithm proposed is entirely based on the work by Amato and Serio, 1991.

2. MATHEMATICAL FRAMEWORK

As far as Fourier spectroscopy is concerned, the relationship which links the spectrum, R, to the measured interferogram, I, is well known to be a cosine Fourier transform:

$$I_k = \frac{1}{T}\int_0^T R(t)cos\left(\frac{k\pi t}{T}\right)dt \tag{1}$$

with T being the maximum wavenumber.
The problem of retrieving the spectrum from the measured interferogram is of course an inverse problem and it is well known that such problems are ill-posed and then give rise to a lot of troubles in finding the solution. In particular, error affecting the data of the inverse problem propagate highly amplified onto the retrieved solution. However the situation of interferometry is luckily different, since the inverse cosine Fourier transform belongs to a particular class of inverse problems for which the propagation of error is well behaved: let σ_I denote the experimental error affecting the interferogram and σ_R the error affecting the retrieved spectrum; then it can be easily shown that

$$\|\sigma_R\|_{L^2} = \|\sigma_I\|_{\ell^2} \tag{2}$$

Eq. (2) shows that no amplification of the error occurs when solving the inverse problem[†] and then no particular care could be taken from the mathematical point of view. However, the very nature of the physical problem determines one more trouble: in fact the astonishing high number of molecular transactions in atmosphere makes that a very long interferogram is needed in order to well represent the spectrum; then the overall error affecting the interferogram increases and Eq. (2) says that the overall error on the retrieved spectrum increases as well, even if not amplified. For this reason it makes sense to find mathematical methods such that the solution of the inverse problem satisfies

$$\|\sigma_R\|_{L^2} \leq \|\sigma_I\|_{\ell^2} \tag{3}$$

Then all tools existing for solving inverse problems can be resorted also for the interferometry problem.

3. REGULARIZATION

In order to simplify the notation, we shall previously make the change of variable $f = t/(2T)$, so that the equation to be solved becomes

$$I_k = 2\int_0^{\frac{1}{2}} R(f)\cos(2k\pi f)\,df \tag{4}$$

The whole following discussion equally applies to Eq. (1), provided that suitable algebraic manipulations are made.

[†] To be more precise, the ill-posed character of the problem depends on the norm chosen, but Eq. (2) is true for norms of practical interest in interferometry.

The most consolidated and effective technique for solving inverse problems is the well known Regularization. In this ambit the problem of the inverse cosine Fourier transform is written as:

$$\min_R \mathcal{L}, \quad \mathcal{L} = \frac{1}{m} \sum_{k=0}^{m-1} \left(I_k - 2 \int_0^{\frac{1}{2}} R(f) \cos 2k\pi f df \right)^2 + \lambda \mathcal{S}(R) \tag{5}$$

where

m is the length of the interferogram sample;

$\mathcal{S}$ is a stabilizing functional;

λ is the regularization parameter, $\lambda > 0$.

The role of the stabilizing functional consists in smoothing the oscillations of the solution due to errors on the interferogram. In general it is assumed

$$S(R) = 2 \int_0^{\frac{1}{2}} \left[\frac{d^p R(f)}{df^p} \right]^2 df \tag{6}$$

where $p \geq 0$.

If we look for the solution in the form

$$R(f) = 2 \left(c_0 + 2 \sum_{i=1}^{m-1} c_k \cos(2k\pi f) \right) \tag{7}$$

problem (5) is written as

$$\min_{c_0,\ldots,c_{m-1}} \mathcal{L}_p, \quad \mathcal{L}_p = \frac{1}{m} \sum_{k=0}^{m-1} \left(I_k - 2 \int_0^{\frac{1}{2}} \left(c_0 + 2 \sum_{i=1}^{m-1} c_i \cos 2\pi i f \right) \cos 2\pi k f df \right)^2 +$$

$$\lambda \int_0^{\frac{1}{2}} 2 \frac{d^p}{df^p} \left[c_0 + 2 \sum_{i=1}^{m-1} c_i \cos 2\pi i f \right]^2 df \tag{8}$$

For the sake of brevity, in the following we shall omit the tedious algebraic manipulations for finding the solution of problem (8). It can be shown that

for the case $p = 0$ the solution is

$$\begin{cases} c_0^{(0)} = \dfrac{I_0}{1 + 2\lambda m} \\ c_k^{(0)} = \dfrac{I_k}{1 + 4\lambda m}, \quad k = 1, \ldots, m-1 \end{cases} \tag{9}$$

for the case $p > 0$ the solution is

$$\begin{cases} c_0^{(p)} = I_0 \\ c_k^{(p)} = \dfrac{I_k}{1 + (2k\pi)^{2p} \lambda m}, \quad k = 1, \ldots, m-1 \end{cases} \tag{10}$$

In Amato and Serio, 1991 it is proved that this method is optimal, as far as convergence to the true spectrum is concerned.

4. CHOICE OF THE REGULARIZATION PARAMETER

Eqs. (9) and (10) give a family of solutions depending on the regularization parameter. As in all inverse problems, its choice is quite often crictical, in the sense that very small variations of the parameter can give quite different solutions. Moreover, it is estremely important to have an objective choice—the parameter is uniquely determined by an algorithm—especially in the case of real-time and in-situ computations.

To our knowledge, the only effective criterion for the choice of the regularization parameter when variance of the input data is unknown is the Generalized Cross Validation criterion (Wahba, 1977). If $X\underline{f} = \underline{d}$ is the general integral equation in discretized form and

$$\min_{\underline{f}} \mathcal{L}, \quad \mathcal{L} = \frac{1}{m}\|X\underline{f} - \underline{d}\|^2 + \lambda \underline{f}^T \Sigma \underline{f}$$

is the functional to be minimized, the GCV criterion consists in minimizing the following functional:

$$\min_{\lambda} V(\lambda), \quad V(\lambda) = \frac{\frac{1}{m}\|(I - A(\lambda))\,\underline{d}\|^2}{\left(\frac{1}{m}\mathrm{Tr}\,(I - A(\lambda))\right)^2}$$

with $A(\lambda) = X(X^TX + m\lambda\Sigma)^{-1}X^T$.

For the problem of interferometry it results

<u>case $p = 0$:</u>

$$X = I \qquad \text{and} \qquad \Sigma = \begin{pmatrix} 2 & 0 & \dots & 0 \\ 0 & 4 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 4 \end{pmatrix}$$

so that

$$A(\lambda) = \begin{pmatrix} \frac{1}{1+2m\lambda} & 0 & \dots & 0 \\ 0 & \frac{1}{1+4m\lambda} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \frac{1}{1+4m\lambda} \end{pmatrix}$$

and

$$V_0(\lambda) = m\frac{\left(1 - \frac{1}{1+2m\lambda}\right)^2 I_0^2 + \left(1 - \frac{1}{1+4m\lambda}\right)^2 \sum_{k=1}^{m-1} I_k^2}{\left[1 - \frac{1}{1+2m\lambda} + \sum_{k=1}^{m-1}\left(1 - \frac{1}{1+2m\lambda}\right)\right]^2} \tag{11}$$

By algebraic manipulations, it can be shown that Eq. (11) can be written in a simpler way as

$$V_0(\lambda) = m\frac{(1+4m\lambda)^2 I_0^2 + 4(1+2m\lambda)^2 \sum_{k=1}^{m-1} I_k^2}{(2m + 4m^2\lambda - 1)^2} \tag{12}$$

The minimum value of $V_0(\lambda)$ is obtained for

$$\lambda = -\frac{(m-1)I_0^2 - 2\sum_{k=1}^{m-1} I_k^2}{4m\left(mI_0^2 - \sum_{k=0}^{m-1} I_k^2\right)} \tag{13}$$

case $p > 0$:

$c_0^{(p)} = I_0$ (see Eq. (10)), so that

$$X = I_{m-1} \qquad \text{and} \qquad \Sigma = \begin{pmatrix} (2\pi)^{2p} & 0 & \dots & 0 \\ 0 & (4\pi)^{2p} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & (2(m-2)\pi)^{2p} \end{pmatrix}$$

and then

$$A(\lambda) = \begin{pmatrix} \frac{1}{1+(2\pi)^{2p}m\lambda} & 0 & \dots & 0 \\ 0 & \frac{1}{1+(4\pi)^{2p}m\lambda} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \frac{1}{1+(2(m-1)\pi)^{2p}m\lambda} \end{pmatrix}$$

so that

$$V(\lambda) = \frac{\frac{1}{m}m^2\lambda^2 \sum_{k=1}^{m-1}\left(\frac{(2k\pi)^{2p}}{1+(2k\pi)^{2p}m\lambda}\right)^2 I_k^2}{\left(1 - \frac{1}{m}\sum_{k=1}^{m-1}\frac{1}{1+(2k\pi)^{2p}m\lambda}\right)^2} \tag{11}$$

The minimum value of $V(\lambda)$ is reached for

$$\sum_{k=1}^{m-1} d_k^2 I_k^2 \sum_{k=1}^{m-1} d_k^2 - \sum_{k=1}^{m-1} d_k^3 I_k^2 \sum_{k=1}^{m-1} d_k = 0 \tag{13}$$

where

$$d_k = \frac{(2k\pi)^{2p}}{(2k\pi)^{2p}m\lambda + 1}$$

5. NUMERICAL EXAMPLE

Before giving a brief example concerning the proposed technique, we note that theoretically the order of differentiation of the stabilizing functional S can be any integral $p \geq 0$. However, if we write Eq. (10) in the equivalent form

$$\lambda = \frac{\sum_{k=1}^{m-1}(I_0^2 - 2I_k^2)}{4m\sum_{k=1}^{m-1}(I_0^2 - I_k^2)} \tag{16}$$

it results in general $\lambda < 0$ which is not allowed. This means that the GCV criterion is not effective in the case $p = 0$. Moreover, no theoretical reason can be invoked in preferring any priori value of $p > 0$ for the stabilizing functional; however numerical experiments on this and other inverse problems show that $p = 2$ represents a good choice in general.

Summarizing, the procedure for finding the radiance spectrum from the interferogram, taking account of the experimental error, goes through the following steps:

a) choose the stabilizing functional by fixing $p = 2$;

b) find the optimal regularization parameter λ by solving the non linear equation (15);

c) calculate the *regularized* interferogram (that is the Fourier coefficients of the radiance function smoothed by the proper amount of regularization) by means of Eq. (10);

d) finally calculate the radiance from the regularized interferogram by usual FFT tools.

In this section we present an example based on a sample spectrum obtained by FASCOD2. The interferogram was calculated on 2049 points. Two different cases are considered: in the first one no error corrupts the simulated interferogram, while in the second one a random noise is simulated, following a normal distribution with variance, σ^2, constant all over the interferogram ($\sqrt{\sigma^2} = 31$, corresponding to ratio signal/noise of about 5000).

In the first case the Generalized Cross Validation criterion gives an optimal value $\lambda = 0$; the corresponding retrieved spectrum is equal to the not regularized one and no smoothing is provided by regularization. In this example the GCV criterion correctly recognizes that no error affects the interferogram.

In the second case the Generalized Cross Validation criterion gives a value $\lambda = 0.268 \cdot 10^{-18}$ and then regularization is effective. The retrieved spectrum is 30% better than the not regularized one ($\lambda = 0$). Figs. 1 and 2 show the true spectrum and spectra retrieved with $\lambda = 0$ (no regularization) and $\lambda = 0.268 \cdot 10^{-18}$ (given by GCV), respectively.

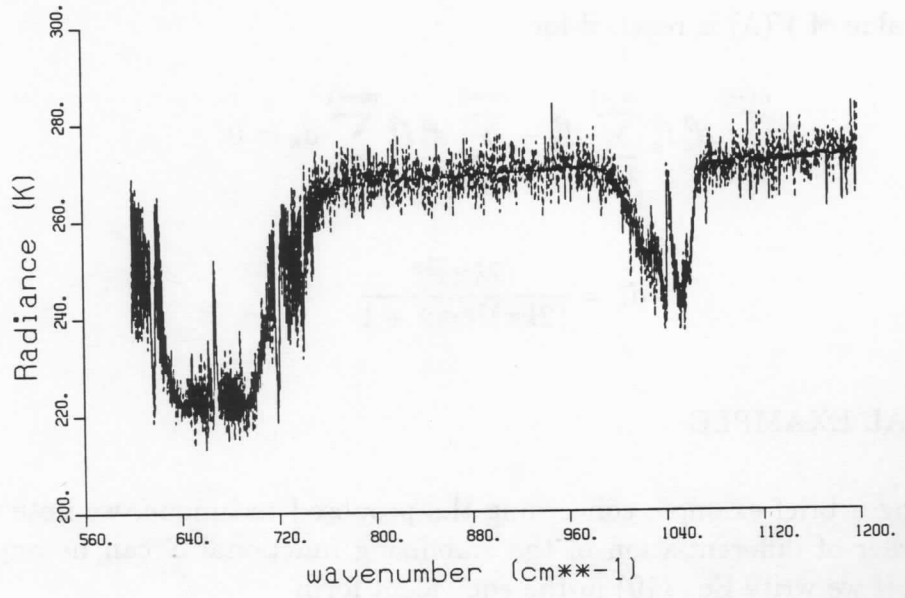

Fig. 1: True spectrum (continuous line) and spectrum retrieved without regularization (dashed line) for the case 5000:1 S/N ratio.

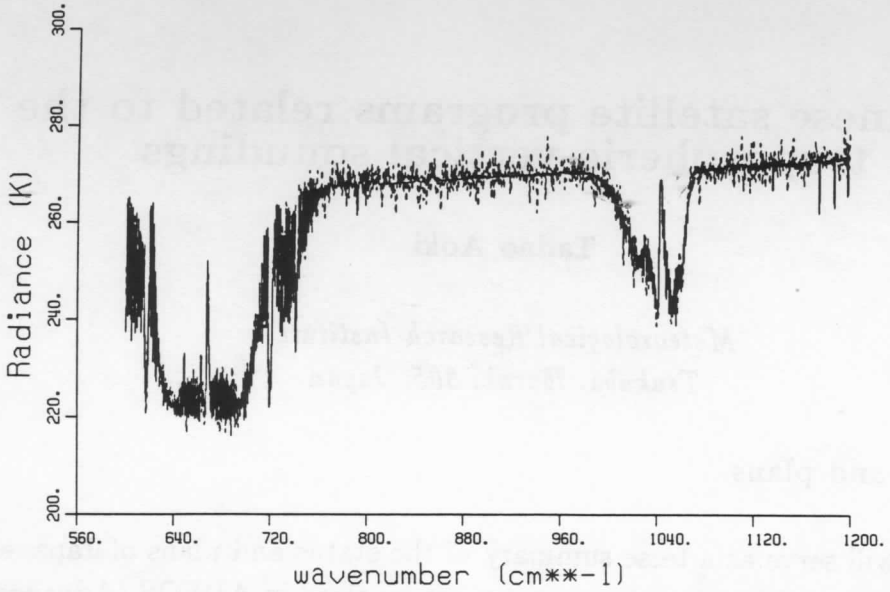

Fig. 2: True spectrum (continuous line) and spectrum retrieved by regularization with λ chosen by GCV (dashed line) for the case 5000:1 S/N ratio.

6. CONCLUSIONS

The present paper dealt with a new method for retrieving radiance from interferometry data based on optimal mathematical techniques. Particular attention is devoted to devise an *algoritm* which is both very fast from a computational point of view and completely objective, in the sense that no parameter has to be tailored by the researcher in order to work. The technique heavy uses FFT, so that its speed of execution can be strongly increased by using devoted chips. A first simple example is given which shows the use and effectiveness of the Generalized Cross Validation criterion. More research is needed in order to analyze the performance of the technique when error and length of the interferogram are increased.

7. REFERENCES

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