Inversion of generalized relaxation time distributions (GRTD) with a L-curve

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From the beginning of the 20th century, retrieving the Relaxation Time Distribution (RTD) has been a challenge in the interpretation of spectra involving relaxation phenomena.

While physicists and electrochemists were the first involved in this questioning, the current revival of Induced Polarization in geophysicists today makes them fully concerned. The inversion of GRTD is a more general approach than the numerous models based on given transfer functions, like the popular Cole-Cole distribution and response. Numerous others provided catalogues of parametric models.

Generally speaking, the decomposition of observed spectra relies on a superposition principle involving elementary Debye relaxation, leading to the expression (given here for conductivity):

$$A_\omega(\omega) = a_\Re - \int_0^{+\infty} \frac{g_\tau(\tau)}{1+i\omega\tau} d\tau + i\omega C\,, \tag{1}$$

where $g_\tau(\tau)$ is the RTD, $a_\Re$ a real constant, and C an empirical constant useful to accommodate the high frequency content (sometimes called the "high frequency dielectric term"). Parametric models are linked with associated distributions, and, in some cases, A_ω is known as well as the linked distribution itself (Cole-Cole in 1941, for instance, provided both functions).

The work introduced here deals with a more general problem, in which the Debye response may be replaced by any kernel like in the expression:

$$A_\omega(\omega) = a_\Re - M \int_0^{+\infty} g_\tau(\tau)\varphi(\omega,\tau)\, d\tau + i\omega C \tag{2}$$

For example, we may use a Warburg decomposition, in which:

$$\varphi(\omega,\tau) = \frac{1}{1+\sqrt{i\omega\tau}} \tag{3}$$

Inversion scheme and example

A triple change of variable is first applied. The two first are classical and transform the equation above into an inhomogeneous Fredholm equation of the second kind:

$$\begin{cases} z = -\log(\omega) \Leftrightarrow \omega = \mathrm{e}^{-z} \\ s = \log(\tau) \Leftrightarrow \tau = \mathrm{e}^{s} \end{cases} \rightarrow \quad A_z(z) = a_\Re - \int_{-\infty}^{+\infty} G_s(s)\Phi(z,s)\, ds + i\mathrm{e}^{-z}C \tag{4}$$

This integral is computed by using Rieman's summation with step Δs, additionally to a spectrum sampling. Then, real and imaginary parts can be split into:

$$A_k^{\Re} = a_\Re - \Delta s \sum_{j=1}^{N_G} \Phi_{kj}^{\Re} G_j \quad \text{and} \quad A_k^{\Im} = -\Delta s \sum_{j=1}^{N_G} \Phi_{kj}^{\Im} G_j + C\mathrm{e}^{-z_k} \tag{5}$$

The third change of variable is applied to impose the required positivity of the RTD. The new unknowns are the G_j' defined by:

$$\forall j \in [\![1, N_G]\!] \quad G_j = \mathrm{e}^{G_j'} \tag{6}$$

This change guaranties the positivity of G_j, but makes the problem fully non linear. We solve it by using Tarantola and Valette generalized least square recursive formalism.

The properties of the kernel make the problem belonging to the ill-posed problem family. To control the regularization factor and damping, we make use of the notion of L-curve), which is no more a canonical L-curve here due to non linearity, but remains usable. The optimum point (low left corner) is determined automatically.

The example given in Fig. 1 illustrates the inversion of a data set by using Warburg decomposition (with the recall of Debye decomposition).

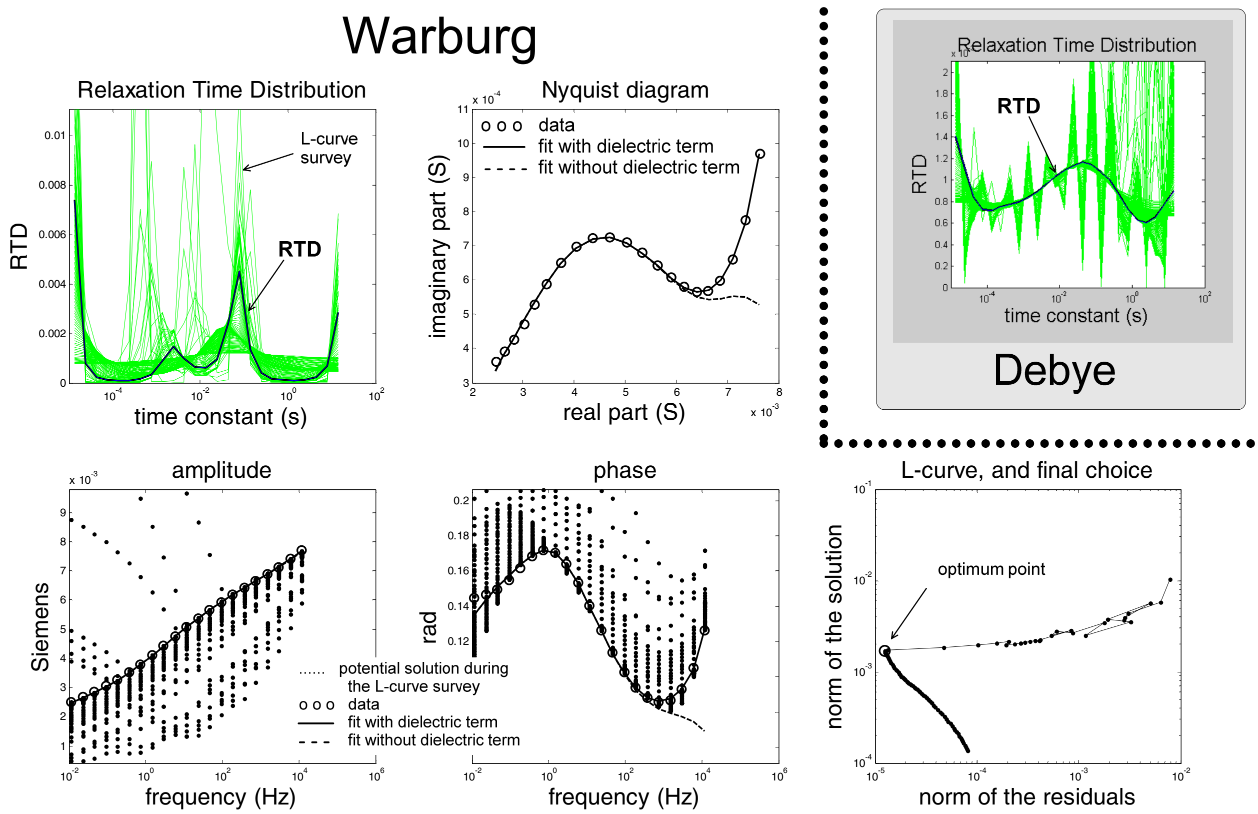

Fig. 1: Aulus data set is relative to the IP response of ancient metallurgic slag heaps. The inversion obtained by using a Debye decomposition leads to a wide bell-shaped distribution (top right), while the Warburg decomposition leads to a more tighten RTD (top left and other plots). The L-curve doesn't look as it should be in the linear case, but permits setting an optimum damping parameter.

The program is available in a beta version by contacting the authors (nicolas.florsch@upmc.fr).