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# Surface NMR Processing and Inversion – III: Inversion

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**SUMMARY**

I present several methods of inverting in-phase and quadrature data for developing a groundwater porosity image that is most consistent with the data. In particular, I employ the principle of maximum entropy and show, with conservative prior estimates of groundwater quantity in the subsurface, the most conservative posterior distribution of groundwater that is consistent with the data.

**Key words:** Surface NMR, groundwater, data fitting.

## INTRODUCTION

Perhaps the final step in obtaining an estimate of the presence of groundwater in the subsurface is through inversion of the recorded data set to obtain a model of groundwater content that is consistent with the data. This is easily done through an SVD inversion (eg), or through an $L_2$ inversion of the groundwater parameters. In this paper, I present an inversion scheme based on the principle of maximum entropy.

## FORWARD MODEL

The forward model operator for groundwater content is the well-known linear operation of the kernel function that operates on the water content model parameters to obtain the in-phase and quadrature components of the free induction decay ($T_2^*$) that are produced from the variation of pulse moments

$$\boldsymbol{g}(\boldsymbol{m}) = \boldsymbol{G} \cdot \boldsymbol{m},$$

where $\boldsymbol{G}$ is the linear forward model kernel operator, and $\boldsymbol{m}$ is the vector of model parameters, ie the water content in the earth (eg, Legchenko and Shushakov, 1998). In a typical $L_2$ inversion, the function to be minimised is the following:

$$\begin{aligned} 2F = {} & (\boldsymbol{g}(\boldsymbol{m}) - \boldsymbol{d}_{obs})' \boldsymbol{C}_D^{-1} (\boldsymbol{g}(\boldsymbol{m}) - \boldsymbol{d}_{obs}) \\ & + (\boldsymbol{m} - \boldsymbol{m}_{prior})' \boldsymbol{C}_m^{-1} (\boldsymbol{m} - \boldsymbol{m}_{prior}), \end{aligned}$$

where $\boldsymbol{d}_{obs}$ are the in-phase and quadrature amplitudes of the signal, $\boldsymbol{C}_D^{-1}$ is the inverse of the data covariance matrix, $\boldsymbol{m}_{prior}$ is the prior model (to be discussed), and $\boldsymbol{C}_m^{-1}$ is the inverse of the model covariance matrix, typically assumed to be some sort of Tikhonov regularisation matrix used to stabilise the inversion. In this paper, we will assume that $\boldsymbol{C}_m^{-1}$ is a simple diagonal matrix of varying model weight $\alpha$, where $\alpha$ is adapted through a line search in order to make the $\chi^2$ value equal to $2N$, $N$ being the number of data points (ie, in-phase and quadrature amplitudes) (Tarantola, 2005).

Alternatively, we may wish an $L_1$ norm on the data space, with an $L_2$ norm on the model space. The objective function then becomes

$$F = \sum_{i=1}^{N} \frac{|g(m_i) - d_i|}{\sigma_i} + (\boldsymbol{m} - \boldsymbol{m}_{prior})' \boldsymbol{C}_m^{-1} (\boldsymbol{m} - \boldsymbol{m}_{prior})$$

and $\sigma_i$ are the standard deviation of the amplitudes, and $\boldsymbol{C}_m^{-1}$ are the uncertainties on the prior models (again, modified by $\alpha$).

As another proposal for the objective function to be minimised, I suggest using the maximum entropy consideration for the balance of the $\chi^2$ distribution. Briefly, the maximum entropy principle states that we wish to maximise the entropy $S$ such that the model parameters agree with the testable information while being non-committal about the distribution of the model parameters themselves. For a given set of model parameters ($\boldsymbol{w}$), we define the Shannon-Jaynes maximum entropy as

$$S = -\sum_{i=1}^{M} m_i \cdot \log\left(\frac{m_i}{\mu_i}\right),$$

where $M$ is the number of model parameters, and $\mu_i$ is the Lebesgue measure. The function to be minimised then becomes

$$F = \frac{1}{2} (\boldsymbol{g}(\boldsymbol{m}) - \boldsymbol{d}_{obs})' \boldsymbol{C}_D^{-1} (\boldsymbol{g}(\boldsymbol{m}) - \boldsymbol{d}_{obs}) - \alpha S,$$

and we interpret $\alpha$ as a Lagrange multiplier used to constrain the minimisation of the chi-squared distribution (Sivia and Skilling, 2006).

## AN EXAMPLE

Let us begin with an example of SNMR data whose in=pahse and quadrature amplitudes have already been found. Figure 1 shows such an example, whereby the $\omega_1$ and $T_{21}^*$ parameters have been obtained to yield amplitudes (with uncertainties) that are most consistent with the recorded time-series data from the experiment (Davis, 2015). Figure 2 shows the in-phase and quadrature kernels for the geophysical model at this location.

Starting with the L2 minimisation function, we need to arrive at a determination of the prior model for the distribution of groundwater in the subsurface, and an estimate of how likely we think the prior model should be. As stated in the abstract, this is the point where we determine our criteria for a conservative estimate of groundwater. I propose as the prior model for groundwater contribution in the subsurface to be

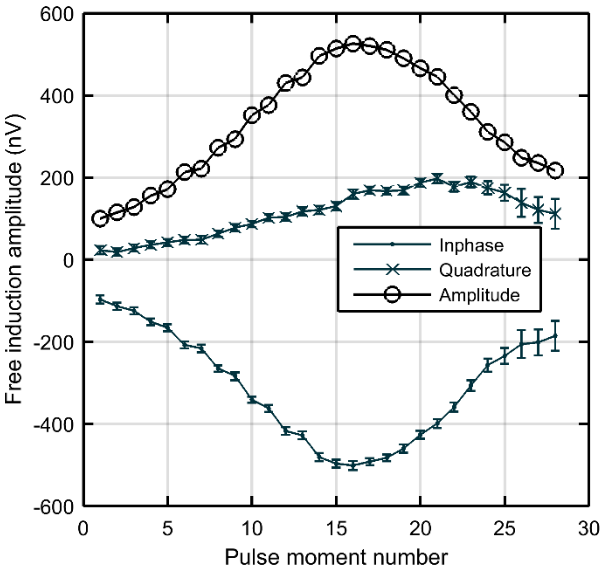


**Figure 1: In-phase and quadrature amplitudes for SNMR experiment, with data uncertainty shown with error bars for every pulse moment.**

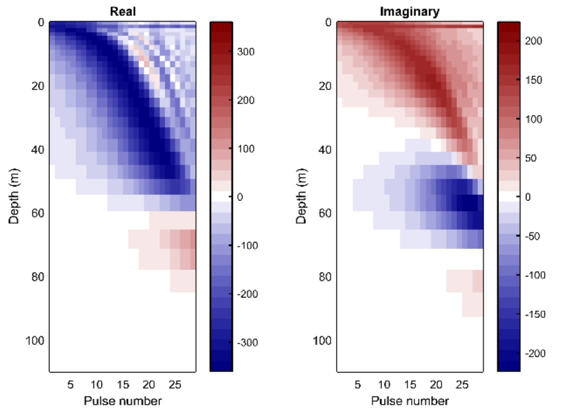


**Figure 2: In-phase (left) and quadrature (right) kernel for the 1D layered earth.**

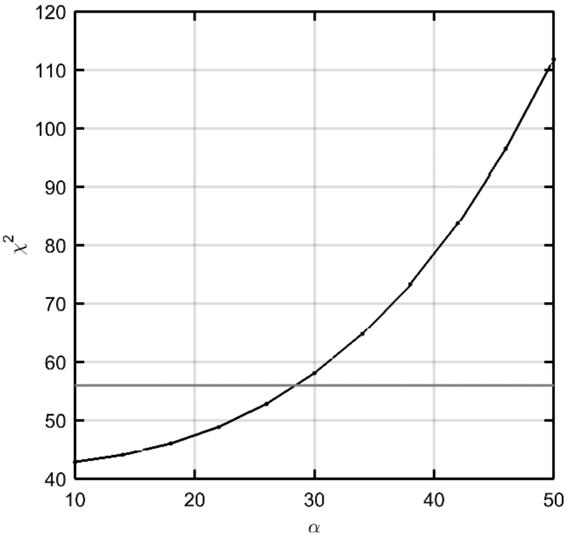


**Figure 3: Variation of $\chi^2$ with $\alpha$ for an $L_2$ norm to the objective function.**

$\boldsymbol{m_{prior}} = \mathbf{0}$. This essentially states that, since we have no idea where groundwater exists, let's say that it doesn't exist at all in the subsurface. This prior model will also be used for the $L_{1,2}$ norm and for the Lebesgue measures in the maximum entropy proposal (except that we take the value of the Lebesgue measure to be very close to zero, since the assumption of maximum entropy ensures positivity).

By conducting the same parameter search on the regularisation value $\alpha$, we see the following 1D groundwater models for each of the different objective functions. Figures 4 and 5 show the inverted in-phase and quadrature amplitudes for each of the model regularisation techniques described here ($L_2$, $L_{12}$ and maximum entropy). In each case, both the in-phase and quadrature components fit the measured data extremely well.

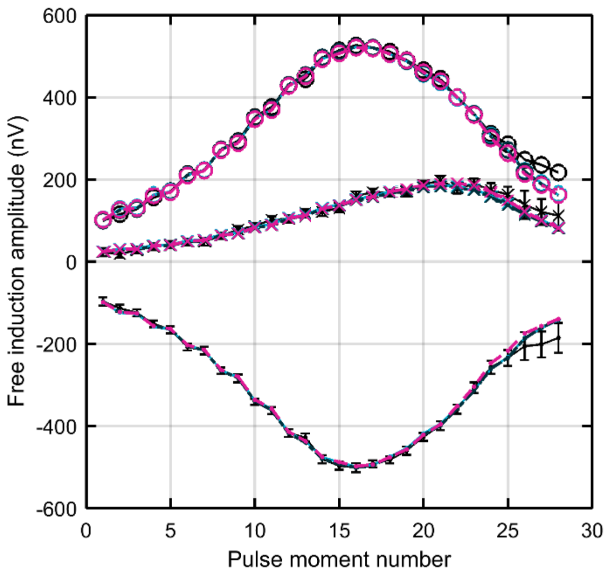


**Figure 4: Modelled in-phase and quadrature amplitudes compared to the measured values (black) for the $L_2$ norm (light blue), $L_{12}$ norm (dark blue) and the maximum entropy (fuchsia) regularisations.**

Also, we see that the inverted groundwater images are extremely similar. This is a good thing, since there is general agreement between the inverted models. Let us consider, for a moment, that our prior distribution of groundwater was $\boldsymbol{m_{prior}} = \mathbf{1}$ for the entire subsurface. The resulting groundwater model, for a new value of $\alpha$ that minimises the $L_2$ norm with the extreme prior, is shown with the thin dashed line in Figure 5. This shows that the data is insensitive to the last few layers of the groundwater model, a fact which could just have easily been garnered from Figure 2. However, our conservative prior model ensures that we do not end up with this confusing situation form the beginning.

The final discussion is about the posterior covariance matrix of the fitting function. Figure 6 shows the posterior covariance matrix for the conservative prior for the $L_2$ norm fitting algorithm. We see, as expected, that the last few model parameters are highly variant with respect to the data, and invariant with respect to any other model parameters. Looking along the main diagonal we see that the models become extremely uncertain below 60 m depth, and that there is some correlation between model parameters at intermediate depths.

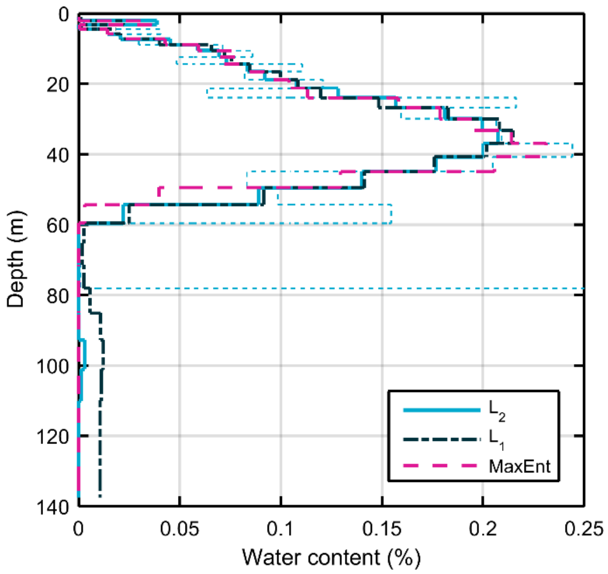


**Figure 5: Resulting groundwater images for the $L_2$ norm (light blue, solid), the $L_{12}$ norm (dark blue, dashed) and the maximum entropy (fuchsia) regularisation parameters.**

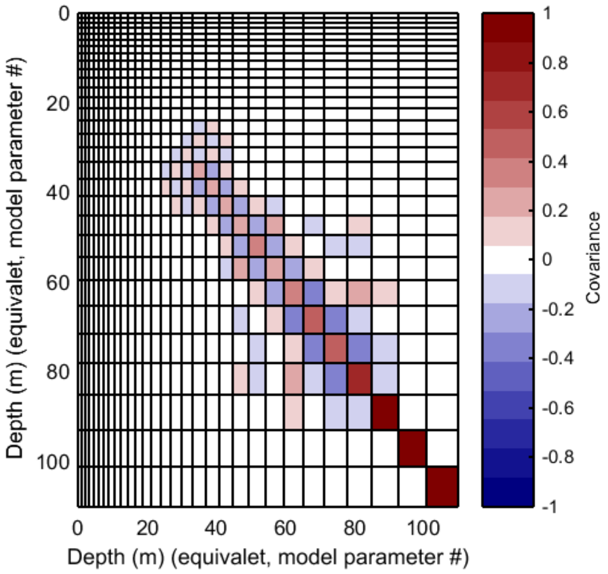


**Figure 6: Posterior covariance matrix for the most probable model of the $L_2$ norm condition. We see that the last few model parameters are highly variant, but with no covariance, while all other parameters are less variant.**

## CONCLUSIONS

In this paper, I have demonstrated a few inversion schemes for groundwater quantity with respect to depth from the in-phase and quadrature components of an SNMR experiment. Specifically, I discussed the $L_2$, and the $L_{12}$ norms on the objective function to be minimised, and demonstrated the use of the maximum entropy principle for groundwater models. Each of these regularisation techniques yield similar groundwater estimates when the regularisation parameter is chosen so that the chi-squared distribution is approximately equal to $N$, the number of data points in the measurement. I have shown that a conservative choice of prior model yields consistent models for each of the regularisations, and that the posterior covariance matrix gives an estimation of the model uncertainty.

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